

DESIGN OF A MONITORING NETWORK FOR
RADIOACTIVE POLLUTANTS IN GROUNDWATER
USING STOCHASTIC OPTIMIZATION

A Thesis Submitted
in Partial Fulfilment of the Requirements
for the Degree of

MASTER OF TECHNOLOGY

by

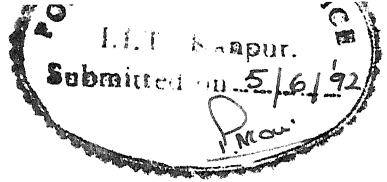
SANJAY DHARAMRAJ DHIMAN

to the

DEPARTMENT OF CIVIL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY
KANPUR

JUNE, 1992

to
my
beloved parents



11

CERTIFICATE

It is certified that the work contained in this thesis entitled "DESIGN OF A MONITORING NETWORK FOR RADIOACTIVE POLLUTANTS IN GROUNDWATER USING STOCHASTIC OPTIMIZATION" by SANJAY DHARAMRAJ DHIMAN (Roll No. 9010321) has been carried out under my supervision, and this work has not been submitted elsewhere for a degree.

June, 1992

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ABSTRACT

A mathematical model linking a solute transport simulation model and a chance constrained, mixed integer programming optimization model for designing an optimal groundwater quality monitoring network is developed.

The optimization model explicitly considers uncertainties of transport simulation and specified reliabilities of predicting the actual concentrations in time and space. The model is evaluated for different degrees of uncertainties in the transport modeling process by introducing cumulative distribution function (CDF) of the actual concentrations as constraints in the optimization model. The nonlinearities due to incorporation of CDF's are removed by using piecewise linearization scheme. The developed model is solved for various degrees of uncertainties and for different reliability values. The solution results clearly show that the optimal well locations are dependent on the degree of uncertainty and the specified reliability values in the prediction of actual concentrations.

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ACKNOWLEDGEMENT

I express my deep sense of gratitude, gratefulness, respect and admiration to my thesis supervisor Dr. Bithin Datta, for the successful completion of my thesis work. I am deeply indebted to him for his keen interest and encouragement. It has been a reviving and rewarding experience for me to work with him. Sincere thanks are also extended to all the faculty members in Hydraulics and Water Resources specialization of Civil Engineering Department for the thought provoking courses received from them during the programme.

I am thankful to the Charutur Vidya Mandal, and the Principal, Birla Vishvakarma Mahavidyalaya for sponsoring me for the M. Tech. programme.

Thanks are due to all my friends and well wishers. My special thanks are due to my brother Vijay and my parents for giving me lot of encouragement and moral support in all my endeavours. Last but not the least, I am thankful to my wife Renu for her profound understanding throughout this research work.

(Sanjay Dhiman)

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CHAPTER 1

INTRODUCTION

1.1 MOTIVATION FRAMEWORK AND OBJECTIVES

There has been an increasing concern throughout the past two decades to protect our groundwater resources from contamination. The water supplied for domestic and agricultural uses may be polluted by any one of the following potential groundwater contamination sources,

- 1) leaky effluent pipe lines,
- 2) toxic chemical waste disposal sites,
- 3) waste water infiltration,
- 4) irrigation run-off infiltration,
- 5) underground fuel storage tanks, and
- 6) unidentified geologic formations.

Identification of groundwater pollution source and monitoring of groundwater quality are essential steps in groundwater quality management. In this study a mathematical model for designing a groundwater quality monitoring network is developed that links a groundwater pollution transport simulation model and an optimization model, explicitly considering uncertainties of transport simulation. To illustrate the performance of this model, tritium is considered as the (radioactive) pollutant.

Nuclear reactors use heavy water as moderator and coolant which results in considerable production of tritium as an activation product. During their normal operation tritium is routinely released into the environment from the reactors through atmospheric and liquid discharge routes, generally within tolerable discharge limits. On release to the environment, tritium ($T_{1/2} = 12.3$ years) being an isotope of hydrogen assimilates readily with water component of the atmospheric, aquatic and biological systems. In case of an accident large quantity of tritium may enter the groundwater system and can impair the use of water.

In contrast with surface water pollution, subsurface pollution is difficult to detect, is even more difficult to control, and may persist for decades. Thus with the growing recognition of the importance of groundwater resources, efforts are increasing to prevent, reduce, and eliminate groundwater pollution. It becomes essential for the water manager to take this responsibility of detecting the harmful contaminants which moves very rapidly in the saturated zone. Concentration contours at different time periods for pollutant disposal from two sites is shown in Figure 1-4. Remedial actions to combat the threat of contamination requires detection of pollution sources and spatial extent of such concentration. It is therefore necessary to design a groundwater quality monitoring network so as to detect and contain the extent of contamination.

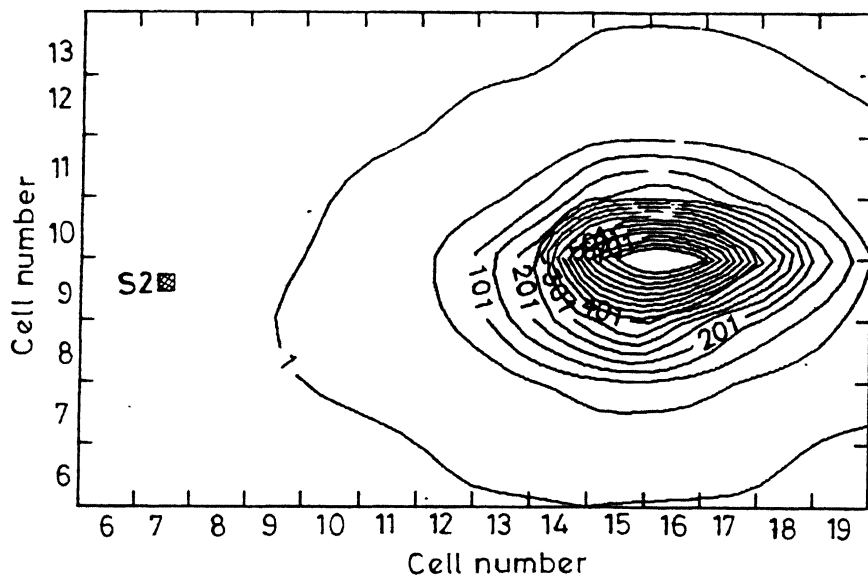


Figure 3. Concentration contours due to pollution source S2 after 4 years

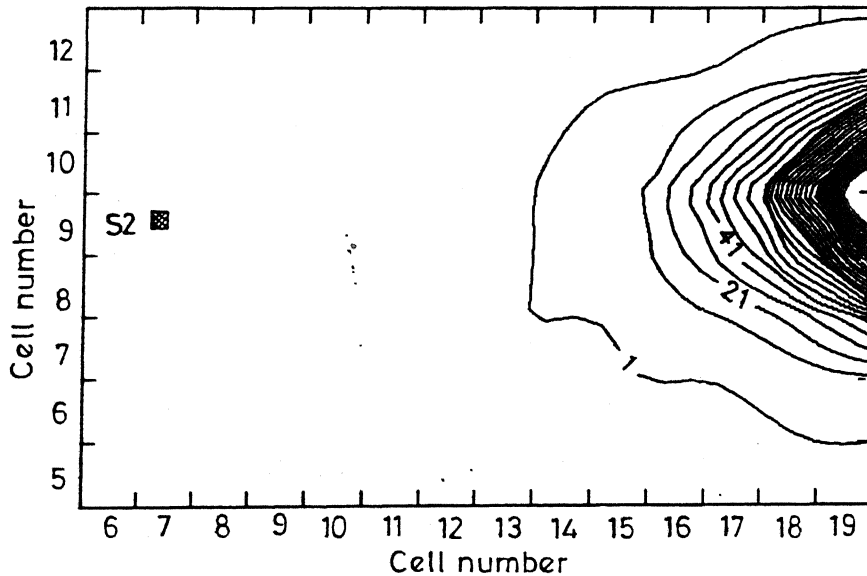


Figure 4. Concentration contours due to pollution source S2 after 6 years

A chance constrained, mixed integer programming model is developed for designing an optimal groundwater quality monitoring network, incorporating uncertainties in the prediction of pollutant movement in the saturated zone. The nonlinearities due to the incorporation of cumulative distribution functions are accommodated through a piecewise linearization scheme. The design of this optimal monitoring network is based on the solutions of two mathematical models : a simulation model for prediction of solute transport in the saturated zone, and an optimization model. The optimization model utilizes the solutions from the simulation model. In particular, the constraints of the optimization model are constructed by incorporating simulation results. The simulation model provides information about the pollutant transport with respect to time and space. The chance constrained optimization model specifies the optimal location of the monitoring wells subject to the maximum limit on the number of such wells.

Parameter estimation uncertainties, heterogeneity of the porous media etc. need to be incorporated while simulating groundwater contamination due to known sources. Optimal design of a monitoring network is a difficult task because, it is difficult to correctly predict the movement of pollutant in groundwater. Also, using large number of groundwater quality monitoring wells is not always physically and/or economically feasible. Therefore there is a necessity of optimal decisions regarding the design of

a monitoring network. These optimal designs should also consider inherent uncertainties in the prediction of pollutant transport.

The primary aim of this work is to design an optimal groundwater quality monitoring network incorporating parameter estimation errors and related inaccuracies in the modeling of the transport process. These errors and uncertainties in modeling may result from errors in observed groundwater table or hydraulic head. These errors and uncertainties in simulation and prediction of solute transport in groundwater can be indirectly accounted for by randomly varying the response matrix, representing influence of pollutant sources upon spatial concentration values evolving over time. The link between the simulation and optimization model is provided through the concentration response matrix.

The role of chance constraints in the optimization model is to introduce a measure of reliability in the predicted concentrations at specified location. Increasing this reliability will result in more conservative prediction of the spatial and temporal distribution of the resulting pollutant concentrations due to known sources. The chance constraints are based on specified values of these reliabilities and the cumulative distribution function (CDF) of the actual value given an estimated value obtained by simulation. The CDF are incorporated in the optimization model. The CDF's of the spatial and temporal values of the concentrations can be obtained by random variations in the estimated inputs to the simulation model, or by random

variations of the response matrix that represents the response of the subsurface saturated zone for given input value of parameters. The general objective of the chance constrained optimization model is to maximize the probability of detecting contamination at locations, where the standard is exceeded, with due weightage given to the degree of exceedences. These exceedence values are computed in terms of the predicted values of concentrations expressed as a function of the specified reliabilities.

1.2 SPECIFIC OBJECTIVES OF STUDY

- (i) Use of USGS (Konikow and Bredehoeft, 1978) computer model for solute-transport simulation.
- (ii) Formulate a chance constrained optimization model linked to a simulation model, for groundwater pollution monitoring network design taking into account uncertainties in the estimation of hydraulic and transport parameters, and other modeling errors.
- (iii) Test the performance of the optimization model for different degrees of parameter uncertainties for specified reliabilities.

1.3 BACKGROUND AND SURVEY OF PREVIOUS WORK

An excellent review of models for groundwater quantity and quality management is given in the classic paper by Gorelick (1983). Much of the following discussion is based on this work with appropriate additions wherever necessary.

1.3.1 Groundwater Modeling

With the help of numerical groundwater flow and transport modeling, it has now become much easier to understand the groundwater systems. Simulation of a groundwater system refers to the formulation and operation of a model whose behaviour assumes the appearance of the actual aquifer behaviour. According to Mercer and Faust (1980), groundwater models, dealing with groundwater flow hydraulics and solute transport can be placed under four general classifications. The models and their application are listed in Figure 5.

In order to take care of uncertainties in the estimation of model parameters the groundwater models can be combined with statistical techniques. Data preparation for the groundwater model first involves determining the boundaries of the model to be modeled, thereafter aquifer parameters and initial data for each grid such as dispersivity, hydraulic conductivity, porosity are to be specified. Care should be taken while using a numerical model as these models are based on a set of simplifying assumptions which limit their use for specific problems only.

1.3.2 Groundwater Management

In the past, numerical simulation models have been used to evaluate groundwater resources. Numerical simulation models that solve groundwater flow or solute transport equation in conjunction with optimization techniques like linear or quadratic programming are powerful aquifer management tools.

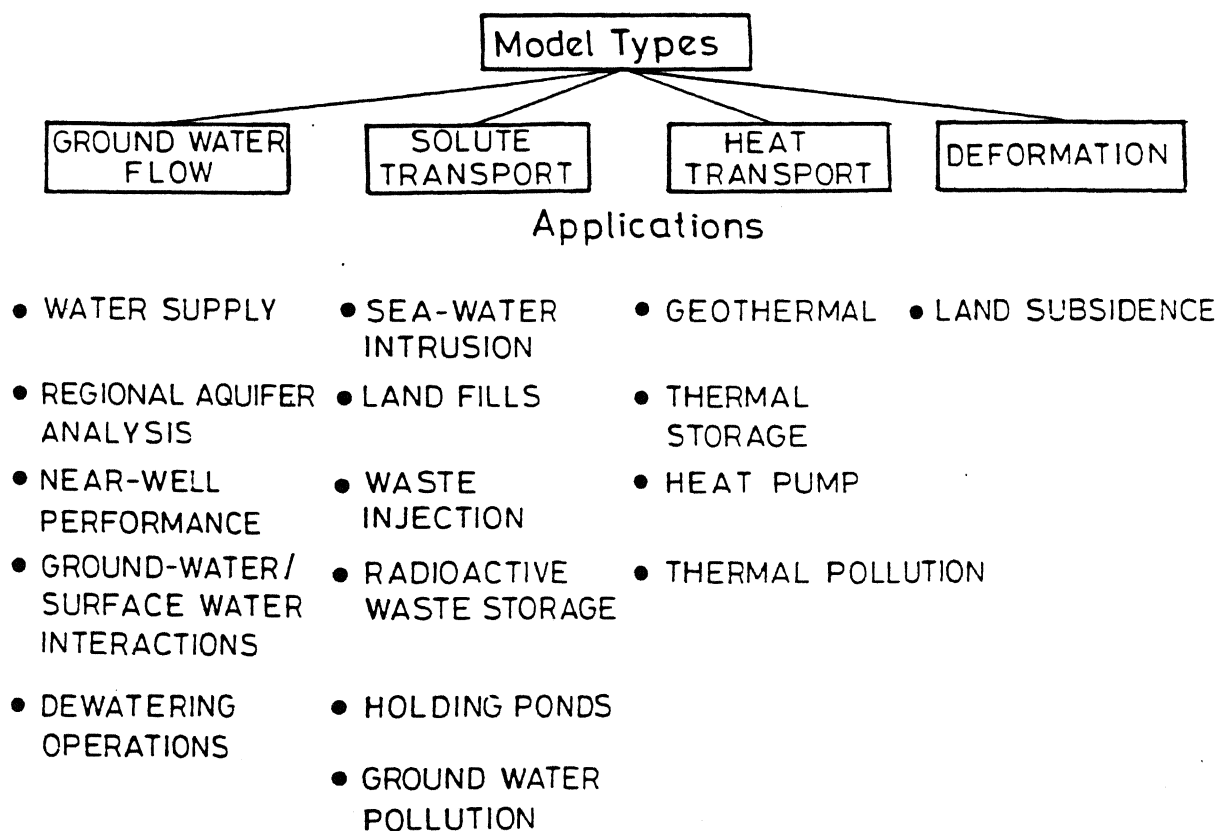


Figure 5. Types of ground-water models and typical applications.(Mercer and Faust,1980)

Simulation as both a method to explore hydrogeologic problems and a tool to predict impacts upon groundwater system will continue to be essential to hydrologists and to water managers. Simulation models are often utilized to explore groundwater management alternatives. In such cases a model is executed repeatedly under various design scenarios which attempt to achieve a particular objective, such as preventing saltwater intrusion, dewatering an excavation area or isolating a plume of contaminated groundwater. In such an approach often physical and operational restrictions are not considered in groundwater management goals. So a joint simulation and management model approach is needed.

Gorelick (1982) classified groundwater hydraulic management models into two basic types

- i) Embedding method
- ii) Response Matrix approach.

The embedding method for the hydraulic management of aquifer uses linear programming formulation that incorporates numerical approximations of the groundwater equations as constraints. In the response matrix approach an external groundwater simulation model is used to develop unit responses. The assemblage of unit responses form the response matrix is included in the management model. In the embedding approach the flow equation are included in the linear programme as constraints and a complete simulation is solved as a part of the optimization model. This helps in

getting a great deal of aquifer information. But it is not always desired to involve all the hydraulic heads over time and space. Hence many of the decision variables and constraints are not necessary in the linear programming or other optimization models.

In response matrix approach solutions to the flow equations serve as constraints. It is very efficient as compared to embedding method as constraints are included only for specified locations and times. So the response matrix approach can be used for large transient systems in an efficient manner.

1.3.3 Groundwater Quality Management

The primary aim of the groundwater quality management model is to minimize the harmful effects of waste disposals by maintaining the water quality standards. The joint use of numerical simulation and optimization models has been applied for groundwater pollutant source management. The need here is to utilize the aquifer for both waste disposal and for water supply. In the following section steady state groundwater quality management model and transient groundwater quality management model are discussed.

1.3.3.A Steady state groundwater quality management model

In steady state groundwater quality management model, the sources of pollution do not change with time, so the problem is only space dependent. Here the storage coefficient is set equal to zero. The time derivatives in the governing equations are also

set equal to zero. In groundwater aquifers steady state conditions normally do not exist.

1.3.3.B Transient groundwater quality management model

In case of transient groundwater quality management the pollution sources occur over both space and time. So the identification of the pollutant source and the time over which the pollution occurs are equally important. The concentration measurements are collected over time at various locations. Although the transient case models are more computationally complex they tend to represent more accurately the aquifer being studied.

1.3.4 Response Matrix Approach in Groundwater Quality Management Problems.

By definition, the concentration response matrix $[R]$ describes the influence of a unit disposal flux on the observation well concentration as a result of the unit pollutant injections at the potential source sites. A groundwater solute transport model is used to simulate these response concentrations for the $[R]$ matrix. These simulation results produce a set of breakthrough curves for each potential disposal site. Each set contains curves for each of the observation wells mapping the concentration resulting from disposal at a particular site.

These curves resemble a unit hydrograph in shape. In actuality, the principle upon which they are based is same. As with unit hydrograph theory, a unit disposal flux is applied to the groundwater system to simulate the resulting response curve.

Each set of curves is then referred to as a suite of breakthrough curves which are used to construct the concentration response matrix [R]. Some of these breakthrough curves are shown in Figure 6.

1.4 GROUNDWATER QUALITY MONITORING NETWORK DESIGN

In order to prove that the groundwater is contaminated or to formulate effective remedial measures, it is essential to test the water samples from the observation wells that are located in the affected area. However economic and other constraints limit the number of wells that can be installed and it becomes essential to design an optimal groundwater quality monitoring network.

With the help of groundwater solute transport simulation model, a likely transport scenario can be obtained. The uncertainties in the estimated parameter values, and the observation errors in hydraulic heads are not incorporated in the simulation model. Moreover for economic feasibility it is not possible to construct a large number of observation wells. It is necessary to apply an optimum criteria to the selection of a monitoring network design. An optimization model can be used to solve these problems. Such an optimization model must consider all physical and managerial constraints and have an explicit objective function.

An approach to the design of a groundwater quality monitoring network was suggested by Meyer and Brill (1988). This method can

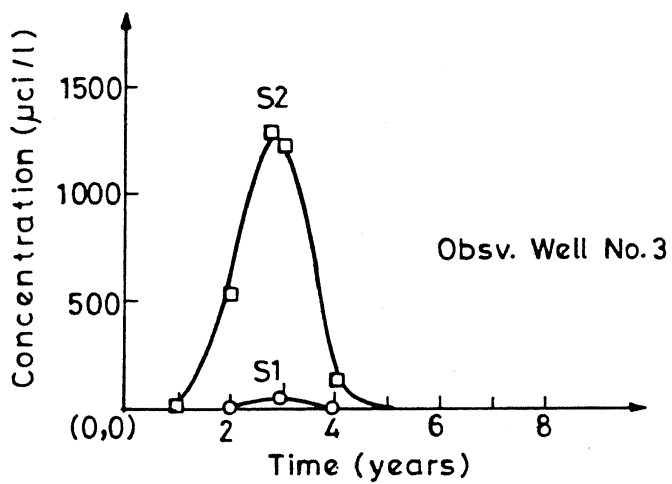
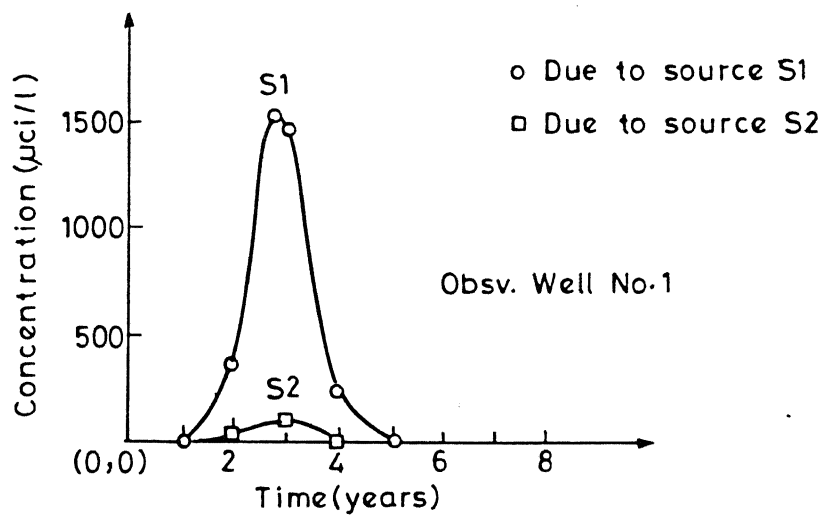


FIGURE 6. A TYPICAL SET OF CONCENTRATION BREAK THROUGH CURVES FOR TWO OBSERVATION WELL LOCATIONS

be used to select a network that maximize probability of detection in the face of uncertainty. While evaluating the performance of the model as proposed by Meyer and Brill (1988) a number of shortcomings were detected, and a new model was suggested by Datta and Purwar (1991). A reverse approach of utilizing the probability of detection for a given monitoring network was suggested by Massmann and Freeze (1987), as part of a larger problem for design of a landfill operation.

The model proposed in this study is capable of designing an optimal groundwater quality monitoring network under condition of uncertainty and incorporates measures of reliability in the prediction of actual concentration at a given location and time. This model is formulated as a mixed integer programming with chance constraints.

Chance constrained model, a particular form of stochastic optimization model has been used in various areas of water resources management. Houck (1979) developed a chance constrained model for reservoir management. Tung (1986) presented a chance constrained model for groundwater quantity management. This model explicitly considers the random nature of transmissivity and storage coefficient, that enable the determination of optimal pumping pattern in a well field subject to a specified system performance reliability. This work also utilizes first order uncertainty analysis for hydraulic conductivity and storage coefficient. However, this model is not applicable to groundwater quality management.

CHAPTER 2

METHODOLOGY

2.1 DESCRIPTION OF THE METHODOLOGY

The proposed chance constrained optimization approach to design an optimal groundwater quality monitoring network under conditions of uncertainty has two major components. The first component involves the use of a groundwater solute transport computer simulation model to simulate pollutant movement from known sources to potential groundwater quality monitoring wells. In the second component simulated concentration data incorporating specified measures of uncertainty in the modeling process are utilised to formulate the chance constrained optimization model for solving a groundwater quality monitoring network design problem.

The proposed model includes a nonlinear objective function and some nonlinear constraints due to cumulative distribution function that are introduced explicitly in the model. However, an equivalent formulation of this nonlinear optimization model is presented and used in this study, using piecewise linearization technique and mixed integer programming. The groundwater solute transport simulation model, the optimization model and the procedure for constructing the response matrix is discussed in detail in the following sections.

2.1.1 USGS Two-Dimensional Flow and Solute Transport Model:

The solute transport in groundwater was simulated using a finite difference based 2-D, numerical model by Konikow and Bredehoeft (1978). The USGS computer model for solute transport combines the groundwater flow equation with the solute transport equation in order to compute the transient changes in reactive/nonreactive solute concentration. The model may be applied to both steady state and/or transient flow problems for one dimensional or two dimensional flows. Its purpose is to identify the change in dissolved chemical concentration in the aquifer at desired locations over time. Due to the process of convection, hydrodynamic dispersion, chemical reactions, adsorption, fluid sources or sinks, and dilution or mixing of the fluid sources, there is change in concentration.

The hydraulic head distribution in the aquifer is simulated by the groundwater flow equation. Pinder and Bredehoeft (1968) derived the following equation to describe the transient two dimensional areal flow through a non-homogeneous, anisotropic confined aquifer by a homogeneous incompressible fluid (using Einstein notation)

$$\frac{\partial}{\partial x_i} \left[T_{ij} \frac{\partial h}{\partial x_j} \right] = S \frac{\partial h}{\partial t} + W \quad i, j = 1, 2 \quad (1)$$

where, T_{ij} = transmissivity tensor, L^2/T ;

h = hydraulic head, L ;

S = Storage coefficient, (dimensionless);

t = time, T ;

$W = W(x,y,t)$, volume flux per unit area (positive for outflow and negative for inflow), L/T; and

x_i, x_j = Cartesian coordinates, L.

If the fluxes, $W(x,y,t)$ deal with direct withdrawal or recharge or a steady leakage into or out of the aquifer, then the following equation is used:

$$W(x,y,t) = Q(x,y,t) - \frac{k_z}{m} (H_s - h) \quad (2)$$

where, Q = rate of withdrawal (+ sign) or recharge (- sign), L/T;

k_z = vertical hydraulic conductivity of the confining layer, streambed, or lakebed L/T,

m = thickness of the confining layer, streambed or lakebed, L; and

H_s = hydraulic head in the source bed, stream, or lake, L.

The derivation from Darcy's law for the average seepage velocity is as follows.

$$V_i = - \frac{k_{ij}}{e} \frac{\partial h}{\partial x_j} \quad (3)$$

where, V_i = Seepage velocity in x direction, L/T;

k_{ij} = hydraulic conductivity tensor, L/T; and

e = effective porosity of the aquifer (dimensionless)

The chemical concentration in the aquifer system is described by solute transport equation. The following is the equation for transient two-dimensional areal transport and dispersion of a given single reactive dissolved chemical species in the flowing groundwater [Gorelick, et al., 1983]

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left[D_{ij} \frac{\partial C}{\partial x_j} \right] - \frac{\partial}{\partial x_i} (C V_i) - \frac{C'W}{eb} - \lambda C, \quad i, j = 1, 2 \quad (4)$$

where,

C = Concentration of the dissolved chemical species; mg/l
 $\mu\text{ ci/l}$;

D_{ij} = dispersion tensor, m^2/d

V_i = average pore water velocity in the direction x_i , m/d ;

b = saturated aquifer thickness; m ;

e = effective aquifer porosity; dimensionless;

C' = solute concentration in fluid source or sink, mg/l or
 $\mu\text{ ci/l}$;

W = volume flux (source) per unit area, m/d ;

λ = first order kinetic decay rate, $1/\text{d}$;

x_i, x_j = cartesian coordinates, m ;

t = time, d .

The first term on the right hand side of equation (4) describes the change in concentration due to hydrodynamic dispersion. The effects of convective transport are shown in the second term on the right hand side and fluid sources and/or sinks are represented by the third term the fourth term shows the effect of radioactive decay on the change in concentration. According to Bear (1972), hydrodynamic dispersion is the macroscopic outcome of actual movements of individual tracer particles through the pores. This includes the process of mechanical dispersion which is dependent on fluid flow through the system and the process of molecular and ionic diffusion which are independent of flow. In the development of the USGS model, the definable contribution of molecular and ionic diffusion to hydrodynamic dispersion is assumed negligible. The dispersion coefficient (D_{ij}) is then defined using

Scheidegger's [1961] equation relating the coefficient to the velocity of ground water flow and to the nature of the aquifer:

$$D_{ij} = a_{ijm,n} \cdot \frac{V_m V_n}{|V|} \quad (5)$$

where: $a_{ijm,n}$ = dispersivity of the aquifer; L;

V_m, V_n = components of velocity in m and n directions respectively, L/T and

$|V|$ = the magnitude of the velocity, L/T.

In addition, Scheidegger (1961) defines the dispersivity tensor in terms of two constants for an isotropic aquifer. The longitudinal and transverse dispersivities of the aquifer (a_L and a_T respectively) are related to the longitudinal and transverse dispersion coefficients (D_L and D_T) as follows :

$$D_L = a_L |V| \quad (6)$$

$$\text{and } D_T = a_T |V| \quad (7)$$

There are numerous assumptions associated with the use of the flow and solute transport equations. These assumptions must be taken into account when applying the USGS solute transport model to an actual field problem. The assumptions summarized by Konikow and Bredehoeft [1978] are as follows:

1. Darcy's law is valid and the only significant mechanism for driving the flow through the system are the hydraulic-head gradients.
2. Porosity and hydraulic conductivity of the aquifer are constant with time and porosity is uniform with space.
3. The velocity distribution is not affected by the gradients of fluid density, viscosity, and temperature.

4. Vertical variations in head and concentration are negligible.
5. The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.
6. Ionic and molecular diffusion contribution to the total dispersive flux are negligible.

The computer model developed by Konikow and Bredehoeft [1978] is based on a rectangular, block-centered, finite difference grid with nodes at the center. This allows for the input of saturated thickness, transmissivity, boundary conditions initial heads and concentrations, observations points, injection or withdrawal wells, and spatially varying diffuse recharge or discharge conditions. Because analytical solution to the flow and solute transport equation's cannot be solved directly due to the variable properties and complex boundary conditions of an aquifer, the model uses an alternating direction implicit (ADI) method to solve the finite difference equations describing the groundwater flow equation and the method of characteristics to solve the solute transport equation.

2.1.2 The Concentration Response Matrix

To avoid the repeatitive use of simulation model and to provide the necessary input to the optimization model the response matrix (Gorelick, 1982) approach has been used. This particular approach is discussed here. The concentration response matrix describes the influence of unit pollutant sources upon concentrations at specified locations over time.

Each simulation for a unit injection rate at the source results in a suite of breakthrough curves at the groundwater

quality monitoring sites. To create other realistic or probable concentration response curves random error terms are added to each element of the response matrix to account for errors in estimation of groundwater field parameters, and other modeling uncertainties.

Each suite of breakthrough curves serves as one column of the concentration response matrix. A complete assemblage of these constitutes the concentration response submatrix for one management period. This single management period response submatrix is called R_1 . Response submatrices representing additional management period's may be developed by staircasing the original response submatrix. The original submatrix R_1 is repeated and shifted down to account for successive periods. The concentration response matrix $[R]$ therefore consists of several submatrices R_1, R_2, \dots, R_p where p represents last management period. The general structure of $[R]$ matrix is displayed in Fig. 7. The time varying pollutant concentrations at the monitoring sites for different injections of pollutants with known concentrations at different management periods are given by

$$[R] [f] = [C] \quad (8)$$

where

$[R]$ the response matrix

$[f]$ the known actual disposal at sources

$[C]$ concentrations at monitoring wells 1 .. n

Therefore once the $[R]$ matrix has been computed using a mathematical groundwater transport simulation model, the resulting concentrations $[C]$ at different times and locations can be obtained using equation (8) for a given $[f]$. This eliminates the

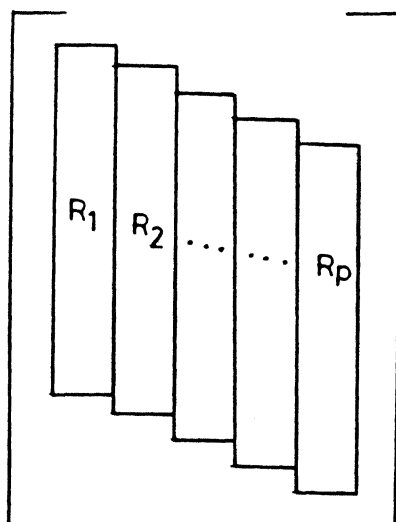


Figure 7. Structure of a concentration response matrix for a ground water quality monitoring wells.

necessity of repeatedly using the simulation model to compute [C] for any new pollutant input condition represented by [f].

2.1.3 Computation of the Response Matrix

Each simulation of a unit injection rate resulted in a suite of breakthrough curves at the monitoring wells. Each suite of breakthrough curves serves as one column of the concentration response matrix. These breakthrough curves (Gorelick, 1982) for a few selected potential observation well locations are shown in Figure 6. These breakthrough curves were constructed for each of the ten potential groundwater quality monitoring well sites for each of the two source locations.

In this study, two pollution sources are considered, therefore, the complete collection of two columns (one for each potential disposal site S_1 and S_2) constitute a submatrix containing the concentration response data for 8 years simulations period at each of ten potential observation well location, 1 through 10. the single management period for constructing the response matrix and for the optimization model is assumed to be of 1 year duration. Each submatrix is shifted down by one management period.

2.1.4 Incorporation of Uncertainties in Solute Transport - Simulation

The response matrix can be utilized for simulating the pollutant migration without using an analytical or numerical simulation model to predict resulting concentration for different sources or input conditions. However, these simulated transport conditions are based only on deterministic conditions, ignoring

the uncertainties in parameter estimations and modeling errors. These uncertainties are incorporated here by random perturbation of the [R] matrix, using statistically generated error terms. Thus the originally computed matrix is assumed to be uncertain and then it is varied by adding randomly generated variables to each element of the matrix. This is done by adding random number generated with specified means and variances. A random error term, ξ is added to each elements of the response matrix [R] to obtain new values for the response matrix [R']

$$[R'] = [R] + [\xi] \quad (9)$$

$$\text{and } [R'] [f] = [C] \quad (10)$$

The random error terms given by each element of $[\xi]$ is defined as

$$[\xi_{ij}] = e_{ij} \sigma + \mu \quad (11)$$

where the generated random variable [e] is sampled from a Normal Distribution with a mean μ equal to zero and standard deviation σ , equal to $\alpha \times R_{ij}$, where α is a fraction.

for $\alpha = 0.25$, and $\mu = 0.0$ equation (11) becomes

$$R'_{ij} = R_{ij} + e_{ij} * (0.25 R_{ij}) \quad (12)$$

A FORTRAN programme for statistical perturbation of the [R] matrix is given in Appendix A.

2.1.5 Computation of the Cumulative Distribution Function of Actual Concentration

The cumulative distribution functions (CDF's) of actual concentrations are computed using statistically generated values of [R'] and utilizing equation 10. For each given [R'] a value of probable concentration at a specified location is generated. For a large set of generated [R'] matrix, a large number of

concentrations are generated statistically. These $\{C\}$ values for a particular location at a specific time period form a sample set of concentration at a location and time, for the same input condition.

The plotting position formulae (or other appropriate methods) can be used to obtain the CDF for actual concentration at a location at a given time. This method is adopted in this study. A typical cumulative distribution function for concentrations at a given location for different degree of uncertainty (α) is shown in Figure 8.

2.1.6 Chance Constrained Optimization Model for Groundwater Quality Monitoring Network Design

A chance constrained optimization model is presented in this section for an optimal design of groundwater quality monitoring network. The role of the chance constraints in the model is to introduce a measure of reliability in the estimated values of predicted concentrations at specified locations. The estimated values of predicted concentration depend upon the degree of uncertainty incorporated.

The optimization model incorporates the cumulative distribution function (CDF) of the actual concentration for each potential groundwater quality monitoring well location for specified management periods. The CDF's of the actual concentrations can be obtained by randomly varying the response matrix, that represents the unit response of the subsurface saturated zone for given input conditions.

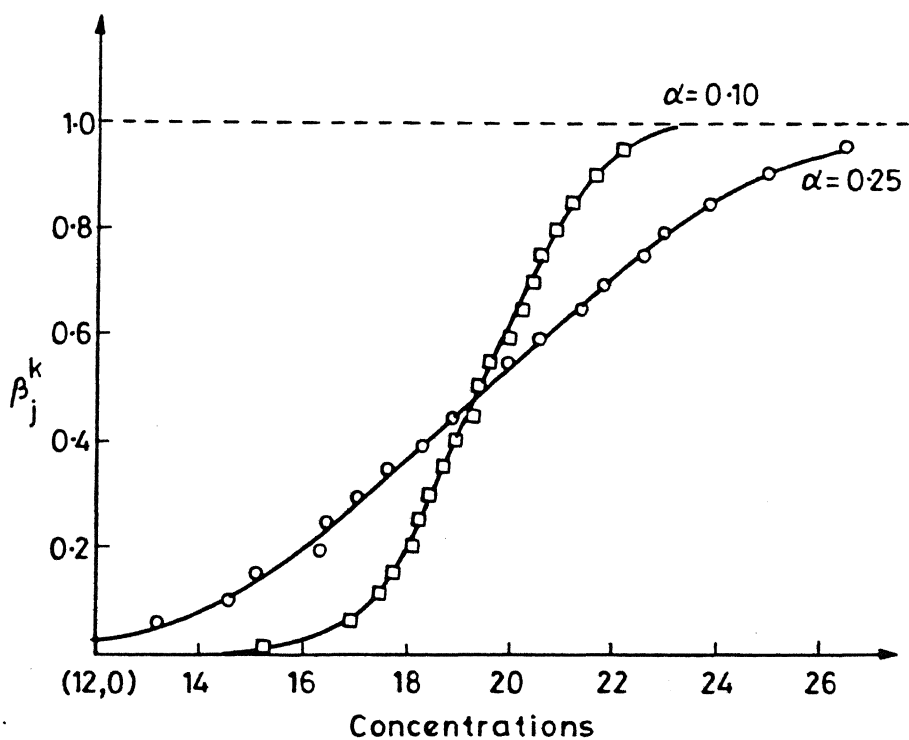


Figure 8 Typical cumulative distribution function for concentrations at a given location for different values of α

The general objective of the chance constrained optimization model is to maximize the probability of detecting contaminations at locations, where a given pollution standard is exceeded. This general objective is mathematically stated in this model as minimization of locationwise sum of the positive difference between the undetected spatial and temporal pollutant concentrations and the contaminant concentration standard, subject to imposed chance constraints.

This nonlinear objective function is converted to linear objective function with suitable modifications in the constraints. The nonlinear constraints due to nonlinear COF's introduced in the model are transformed to linear constraints by using piecewise linearization technique. The resulting mixed integer programming model is solved using LINDO (Linear Interactive Discrete Optimizer).

A chance constrained mixed integer programming model for the monitoring network design can be stated as:

$$\text{Minimize: } Z = \sum_{k \in K'} \sum_{j \in J'} (x_j^k - S_j) (1 - y_j) \quad (13)$$

subject to :

$$\sum_{j \in J} y_j \leq P \quad (14)$$

$$P [C_j^k \leq x_j^k] = \beta_j^k, \text{ for } \forall j \in J \quad (15)$$

$$\beta_j^k \geq \gamma_j^k \quad \forall j, \forall k \quad (16)$$

$$x_j^k \geq 0 \quad (17)$$

$$y_j = (0, 1) \quad (18)$$

The following notation are used.

- x_j^k = probable concentration at potential monitoring site j at management time period k , expressed as a function of reliability β_j^k .
- C_j^k = actual concentration at site j at management period k .
- S_j = acceptable standard concentration at potential monitoring site j .
- \in = belonging to the set
- y_j = a decision variable indicating if a monitoring well is to be installed at site j , a value of 1 indicating installation.
- P = maximum number of wells permitted for the entire monitoring network
- \forall = for all values of
- $F_{jk}^{-1}(\cdot)$ = inverse CDF for the predicted concentrations at site j at management time period k .
- β_j^k = probability that the actual concentration at site j at management time period k will not exceed a particular predicted value.
- γ_j^k = a specified value of reliability denoting the required probability that a predicted value of concentration at site j at time period k will not be exceeded.
- J, K = the set of possible value of j & k .
- J', K' = subsets of J and K containing those values of j & k for which $(x_j^k - S_j)$ are positive.

In the above formulation the objective function minimizes the sum of the positive differences between predicted concentrations at potential monitoring sites and the imposed concentration limit or standard at all potential monitoring sites where a monitoring well is not to be installed according to the solution of the model.

This objective function is nonlinear due to the product of two decision variables x_j^k and y_j occurring in this function. Also it is not efficient to determine externally, all the sites where the concentration standard is exceeded at one or more management period.

Constraint (14) limits the total number of monitoring wells to less than or equal to a permissible maximum value of P . Constraint set (15) defines the probability or the reliability that the actual concentration at site j and management period k will not exceed a particular value. Constraint set (16) relates these probabilities to the specified reliability value γ_j^k .

Constraint set (18) denotes that y_j are (0,1) decision variables, a solution value of y_j equal to zero will mean that a monitoring well is not to be installed at site j , while a value of y_j equal to 1 will specify that a well is to be installed at site j .

The chance constraint set (15) can be replaced by an equivalent constraint

$$x_j^k = F_{jk}^{-1}(\beta_j^k) \quad \forall j \in J \quad (19)$$

Here x_j^k is expressed as a function of the probability that the

actual value of the concentration at site j and management period k will not exceed a certain predicted value. This value can be obtained from the CDF's of the actual concentrations, that are computed by considering the uncertainties in the estimation of actual concentrations.

The above mentioned model is difficult to solve due to the nonlinearity of the objective function and also due to the need to identify the subsets J' and K' . Also the solution is further complicated by the decision variable y_j , which can take only integer (0, 1) values. Therefore, this model is modified as follows to convert it into a linear, mixed integer programming model. The modified model can be stated as

$$\text{Minimize: } Z = \sum_{k \in K} \sum_{j \in J} D_j^k \quad (20)$$

subject to :

$$D_j^k \geq x_j^k - S_j - My_j \quad \forall j, \forall k \quad (21)$$

$$\sum_{j \in J} y_j \leq P \quad (22)$$

$$x_j^k = F_{jk}^{-1}(\beta_j^k) \quad \forall j \in J \quad (23)$$

$$\beta_j^k \geq \gamma_j^k \quad (24)$$

$$D_j^k, x_j^k \geq 0 \quad (25)$$

$$y_j = (0, 1) \quad (26)$$

The additional notation used is, M = a positive large real number. Due to the introduction of constraint set (20) the original objective function (13) can be converted to an equivalent linear objective function that also ensures that only the positive

deviations i.e. positive value of $x_j^k - S_j$ values are included in the objective function, at potential locations where a monitoring well is not to be installed.

The product of two decision variables occurring in the objective function (13) does not appear in the new objective function (20). the large value of M ensures that whenever y_j is nonzero, D_j^k can take values equal to zero. Also, when $x_j^k - S_j$ is negative, even if y_j is equal to 1, D_j^k can take a value equal to zero. The formulation is still nonlinear because the CDF's of actual concentrations are nonlinear functions of β_j^k . To overcome this problem, piecewise linearization scheme is used to linearize the CDF's. Figure 9 shows a typical CDF linearized by three straight lines. The piecewise linearized CDF's are introduced in the optimization model using suitable constraints. The resulting model can be solved as a mixed integer programming model. The piecewise linearization scheme is explained in details in the following section.

The piecewise linearized CDF's are represented in the optimization model with the following new constraints, assuming that three linearized pieces are used to linearize a particular CDF, in the range of interest.

$$\beta_j^k \leq m_1^{jk} x_j^k + C_1^{jk} \quad \forall j, \forall k \quad (27)$$

$$\beta_j^k \leq m_2^{jk} x_j^k + C_2^{jk} \quad \forall j, \forall k \quad (28)$$

$$\beta_j^k \leq m_2^{jk} x_j^k + C_2^{jk} \quad \forall j, \forall k \quad (29)$$

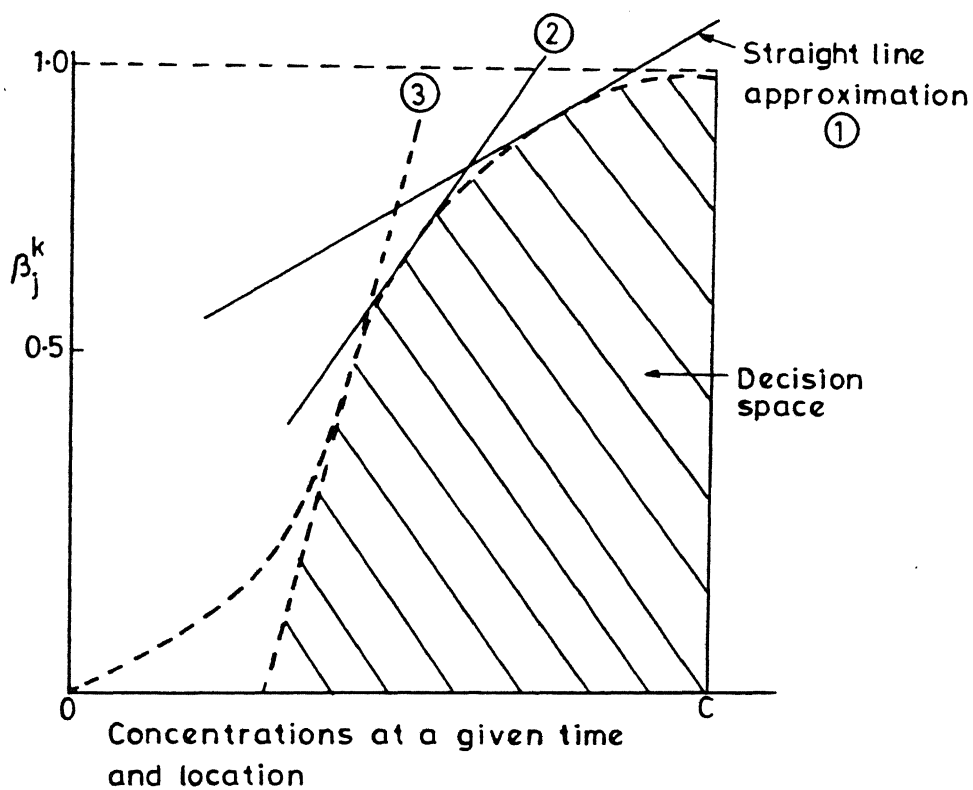


Figure 9 Piece wise linearization scheme for the decision space defined by the cumulative distribution function of the pollutant concentrations.

where

$m_1^{jk}, m_2^{jk}, m_3^{jk}$ = coefficients of the linear equation representing a linearized portions of a CDF for a given j and k .
 $c_1^{jk}, c_2^{jk}, c_3^{jk}$ = constant terms in the linearizing equations for given values of j and k .

It is not required to consider the values of (β_j^k) less than 60 or 70% so that the decision space can be safely assumed to remain convex, guaranting an optimal solution. The objective function (20) together with the constraints (21) - (26) is the new optimization model for solving the monitoring network design problem. This model explicitly incorporates the CDF's of actual concentration at different locations and management periods.

CHAPTER 3

SPECIFIC APPLICATION AND DISCUSSION OF RESULTS

3.1 STUDY AREA

The study area comprises of a portion of an aquifer. This study area is of irregular geometry with impermeable boundaries on the left and right, and non uniform steady flow from top to bottom of the (Figure 10). The finite difference grid applied to the system is shown in Figure 10. The two sources of pollution S_1 and S_2 as well as the potential observation well locations are shown in Figure 11. The coordinates of observation well locations are given in Table 1. The aquifer is assumed to be homogeneous and isotropic. The aquifer parameter values are given in Table 2.

A radioactive pollutant (Tritium, H^3 , $T_{1/2} = 12.3$ years) is assumed to enter the groundwater system from sources S_1 and S_2 . The actual disposal of the pollutant takes place during the first 4 management period only. The pollutant fluxes from sources S_1 and S_2 for four management periods are given in Table 3. In this study the maximum permissible concentration for tritium is taken as 3 $\mu\text{Ci/l}$ for all locations.

3.2 DISCUSSION OF RESULTS

The proposed optimization model was solved for a number of scenarios, with different degrees of uncertainties, and with different values of P and the reliabilities. Table 4 shows the

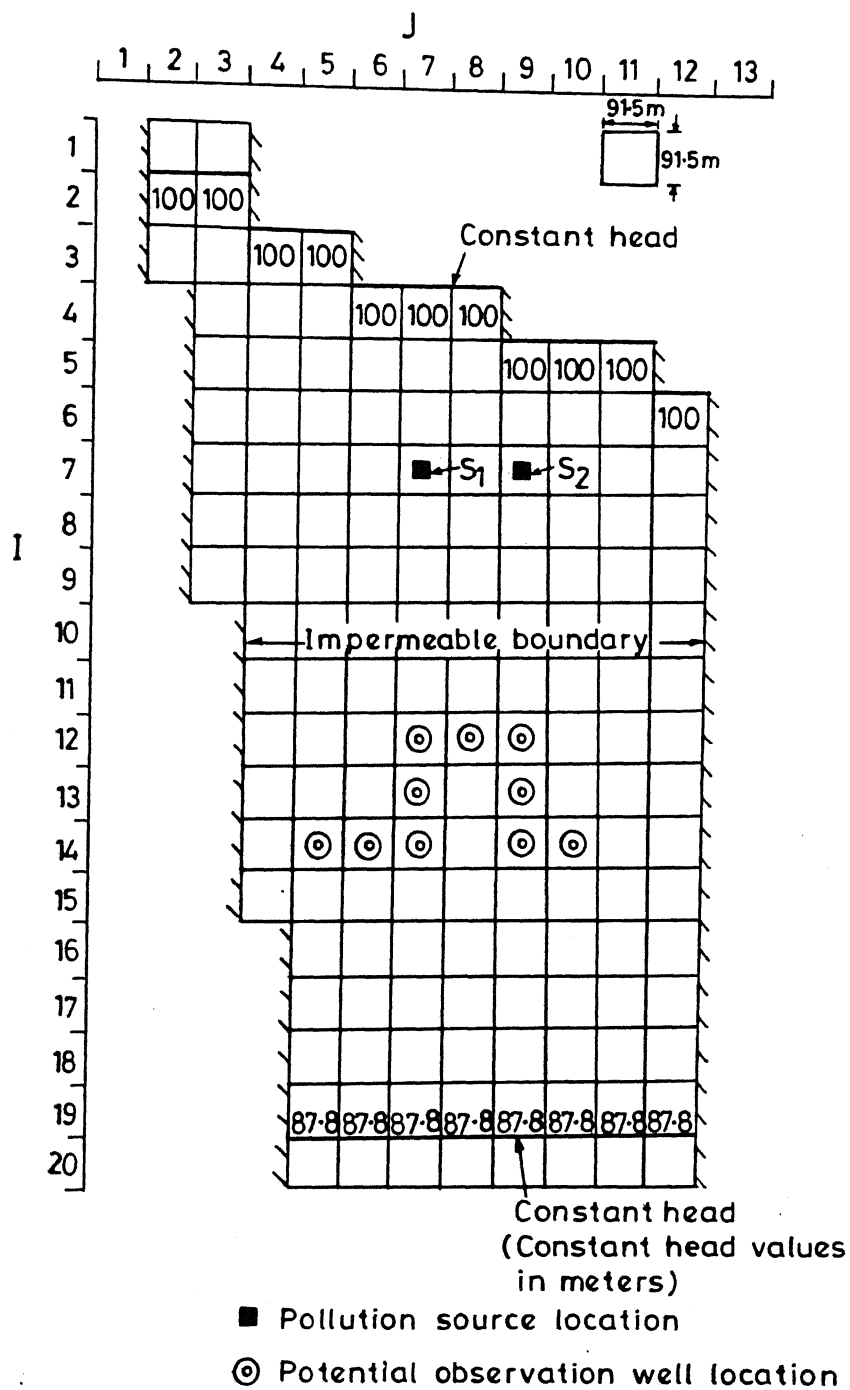
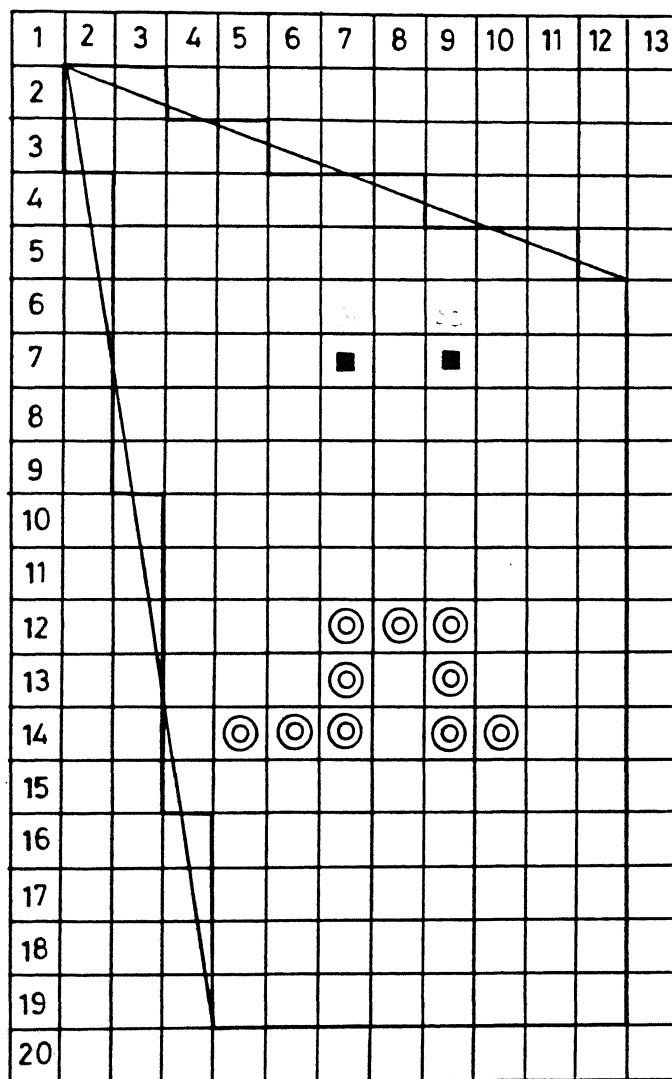


Figure 10 Aquifer study area with steady non-uniform regional flow field



■ Pollution source location

⊙ Potential observation well location

Figure 11 Potential observation well locations

Table 1: Potential Groundwater Quality Monitoring
Well Locations.

Well No.	Grid Coordinates (I,J)
1	(12, 7)
2	(12, 8)
3	(12, 9)
4	(13, 7)
5	(13, 9)
6	(14, 5)
7	(14, 6)
8	(14, 7)
9	(14, 9)
10	(14, 10)

Table 2: Aquifer Parameter values.

Initial Concentration	0.0 μ ci/l
Aquifer thickness	30.5 m
Effective Porosity	0.2
Longitudinal dispersivity	7.625 m
Transverse dispersivity	3.05 m
Hydraulic Conductivity	13 m/day

Table 3: Actual Disposal Fluxes.

	Site No.	Actual Disposal Flux ($\mu\text{Ci/s}$)
Year 1	S1	0.01
	S2	0.01
Year 2	S1	0.01
	S2	0.0
Year 3	S1	0.005
	S2	0.010
Year 4	S1	0.0
	S2	0.005

Table 4: Solution Results of the Optimization Model.

α	β_j^k	S_j	P	Objective function value	Optimal solution in terms of well location
0.1	0.75	3	1	202.9	1
			2	160.09	1,4
			3	118.90	1,4,9
			4	82.49	1,4,8,9
			5	47.52	1,3,4,8,9
			6	19.519	1,3,4,5,8,9
			7	0.5247	1,2,3,4,5,8,9
			8	0	1,2,3,4,5,7,8,9
			9	0	1,2,3,4,5,7,8,9
			10	0	1,2,3,4,5,7,8,9
0.1	0.8	3	1	207.63	1
			2	164.18	1,4
			3	121.41	1,4,9
			4	84.2	1,4,8,9
			5	48.52	1,3,4,8,9
			6	19.876	1,3,4,5,8,9
			7	0.6075	1,2,3,4,5,8,9
			8	0	1,2,3,4,5,7,8,9
			9	0	1,2,3,4,5,7,8,9
			10	0	1,2,3,4,5,7,8,9
0.1	0.9	3	1	219.75	1
			2	173.56	1,4
			3	127.42	1,4,9
			4	88.87	1,4,8,9
			5	57.03	1,3,4,8,9
			6	20.729	1,3,4,5,8,9
			7	0.7729	1,2,3,4,5,8,9
			8	0	1,2,3,4,5,7,8,9
			9	0	1,2,3,4,5,7,8,9,10
			10	0	1,2,3,4,5,7,8,9,10
0.1	0.95	3	1	227.19	1
			2	178.96	1,9
			3	131.201	1,4,9
			4	91.81	1,4,8,9
			5	52.75	1,3,4,8,9
			6	21.57	1,3,4,5,8,9
			7	1.0	1,2,3,4,5,8,9
			8	0	1,2,3,4,5,7,8,9
			9	0	1,2,3,4,5,7,8,9,10
			10	0	1,2,3,4,5,7,8,9,10

Table 4 (Continued).

α	β_j^k	S_j	P	Objective function value	Optimal solution in terms of well location
0.25	0.75	3	1	239.39	4
			2	187.07	1,4
			3	142.58	1,3,4
			4	98.34	1,3,4,8
			5	60.07	1,3,4,8,9
			6	24.07	1,3,4,5,8,9
			7	1.87	1,2,3,4,5,8,9
			8	0.214	1,2,3,4,5,7,8,9
			9	0	1,2,3,4,5,7,8,9,10
			10	0	1,2,3,4,5,7,8,9,10
0.25	0.90	3	1	251.10	1
			2	197.05	1,4
			3	150.10	1,3,4
			4	104.26	1,3,4,8
			5	63.75	1,3,4,8,9
			6	25.62	1,3,4,5,8,9
			7	2.40	1,2,3,4,5,8,9
			8	0.39	1,2,3,4,5,7,8,9
			9	0	1,2,3,4,5,7,8,9,10
			10	0	1,2,3,4,5,7,8,9,10
0.25	0.95	3	1	266.8	4
			2	209.2	1,4
			3	159.34	1,3,4
			4	111.20	1,3,4,8
			5	68.13	1,3,4,8,9
			6	27.53	1,3,4,5,8,9
			7	3.05	1,2,3,4,5,8,9
			8	0.649	1,2,3,4,5,7,8,9
			9	0	1,2,3,4,5,7,8,9,10
			10	0	1,2,3,4,5,7,8,9,10

results corresponding to optimal design of network for groundwater quality monitoring. Here α refers to the degree of uncertainty for the corresponding CDFs of actual concentrations, β_j^k refers to the probability that the actual concentration will not exceed a particular predicted value at site j and time period k . P refers to the maximum number of wells permitted to be installed for groundwater quality monitoring. S_j refers to the allowable limit of the pollutant concentration at site j .

Figures 12 through 21 shows optimal observation well locations obtained as solution to the model for $\alpha = 0.1$, $\beta_j^k = 0.75$, $S_j = 3 \mu\text{ci/l}$ for all j 's with P varying from 1 to 10. Similarly Figures 22 through 31 shows optimal well locations obtained as solution to the model for $\alpha = 0.25$, $\beta_j^k = 0.75$, $S_j = 3 \mu\text{ci/l}$ for all values of j 's with P varying from 1 to 10.

Increasing the reliability from 0.75 to 0.95 for a given degree of uncertainty (α), will result in a more conservative prediction of the spatial and temporal distribution of the pollutant concentration due to known sources. Figure 32 shows the optimal well location obtained as solution to the model for $\alpha = 0.1$, $\beta_j^k = 0.95$, $P = 2$. Figure 33 similarly shows the optimal well location obtained as solution to the model for $\alpha = 0.25$, $\beta_j^k = 0.9$, and $P = 1$.

These results clearly demonstrate that i) the degree of uncertainty (α) in the CDF's of actual concentration and ii) the explicitly stated reliability of the predicted concentrations β_j^k significantly affect the solution obtained from the optimization model. A measure of the degree of uncertainty is given by α

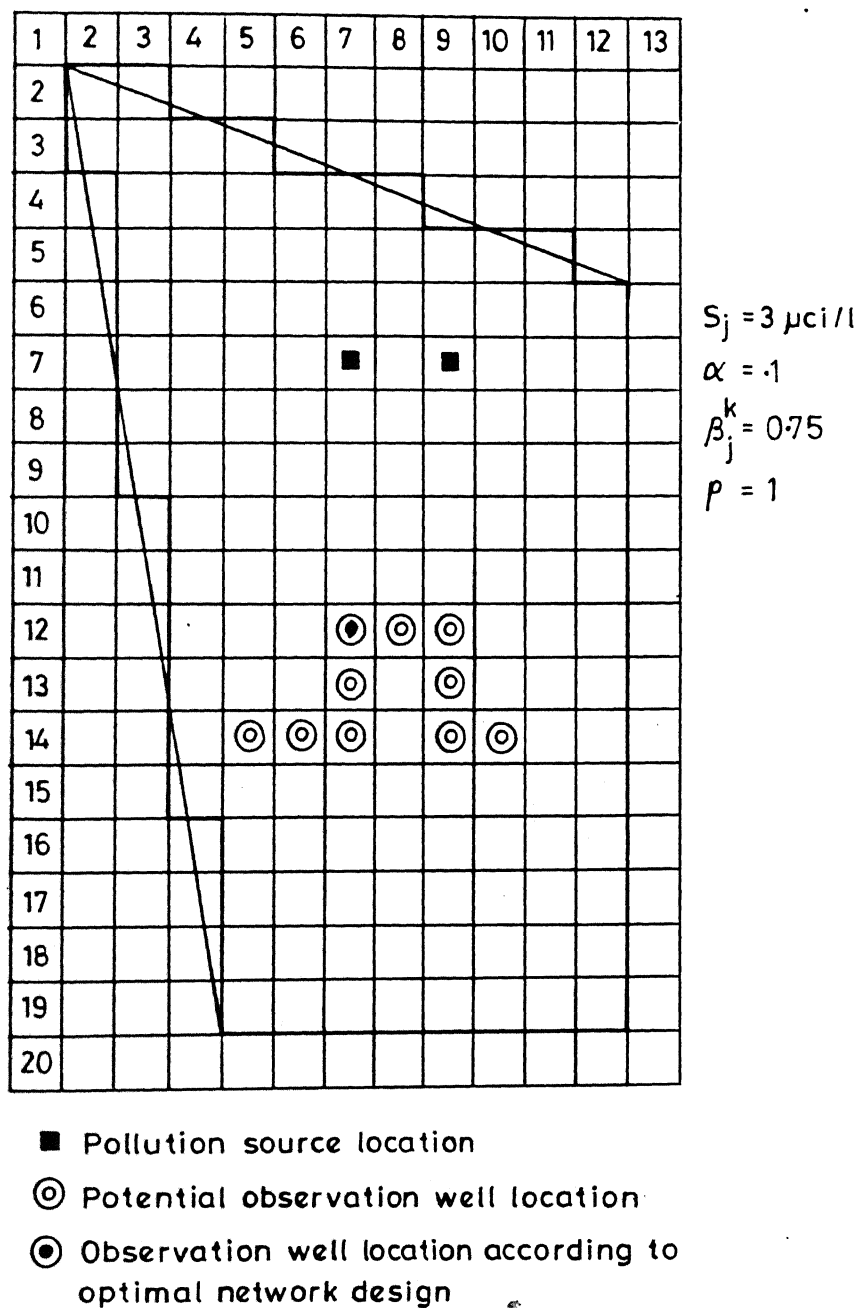


Figure 12 Optimal observation well locations obtained as solution to the model

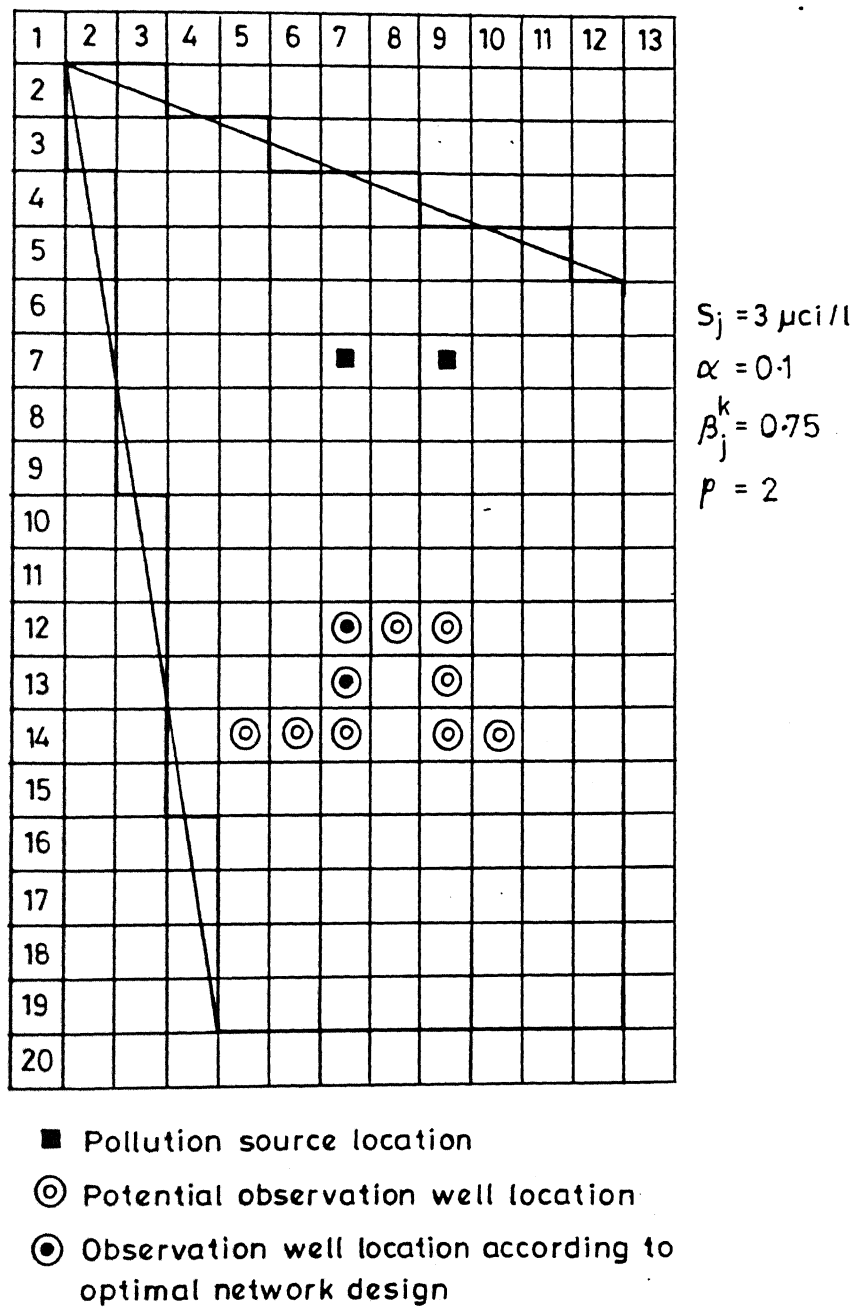


Figure 13 Optimal observation well locations obtained as solution to the model

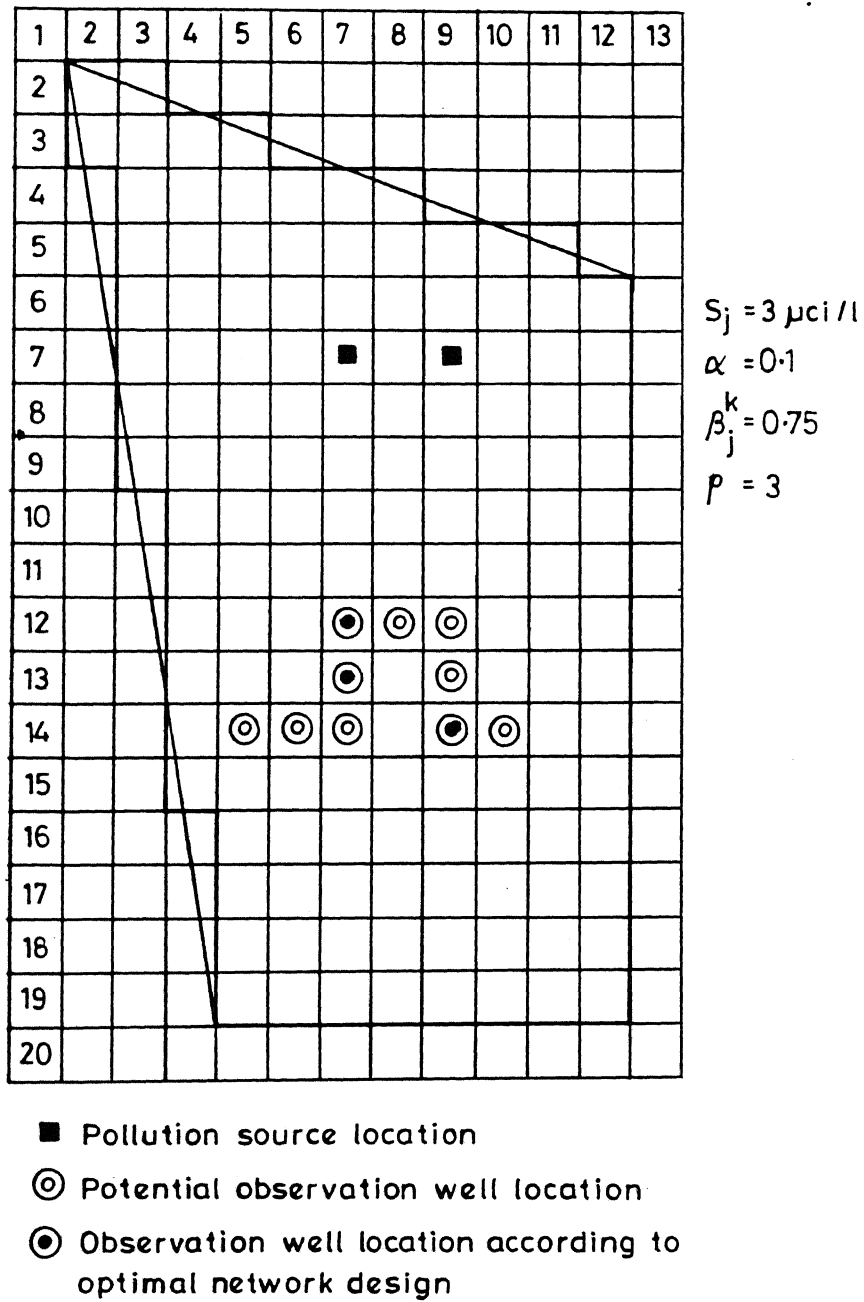


Figure 14 Optimal observation well locations obtained as solution to the model

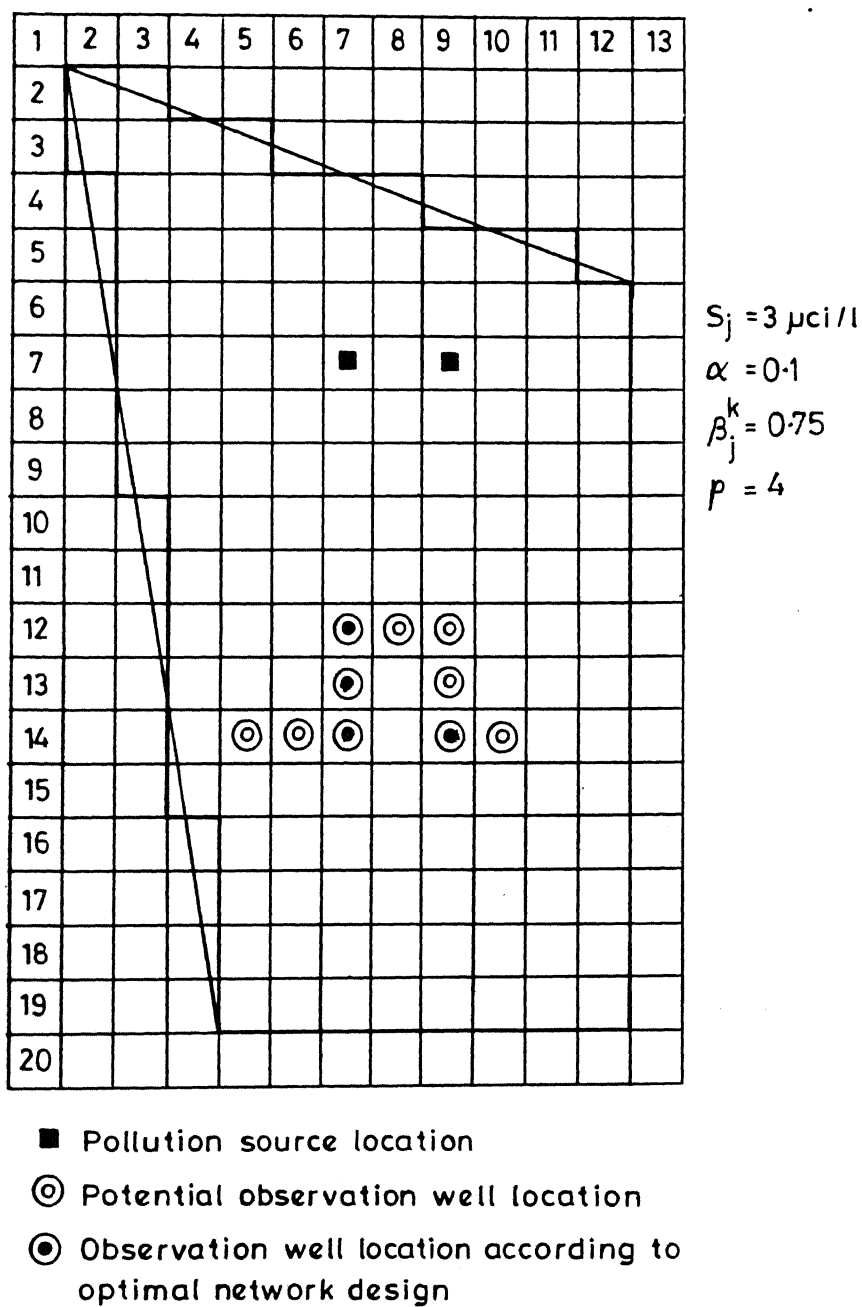


Figure 15 Optimal observation well locations obtained as solution to the model

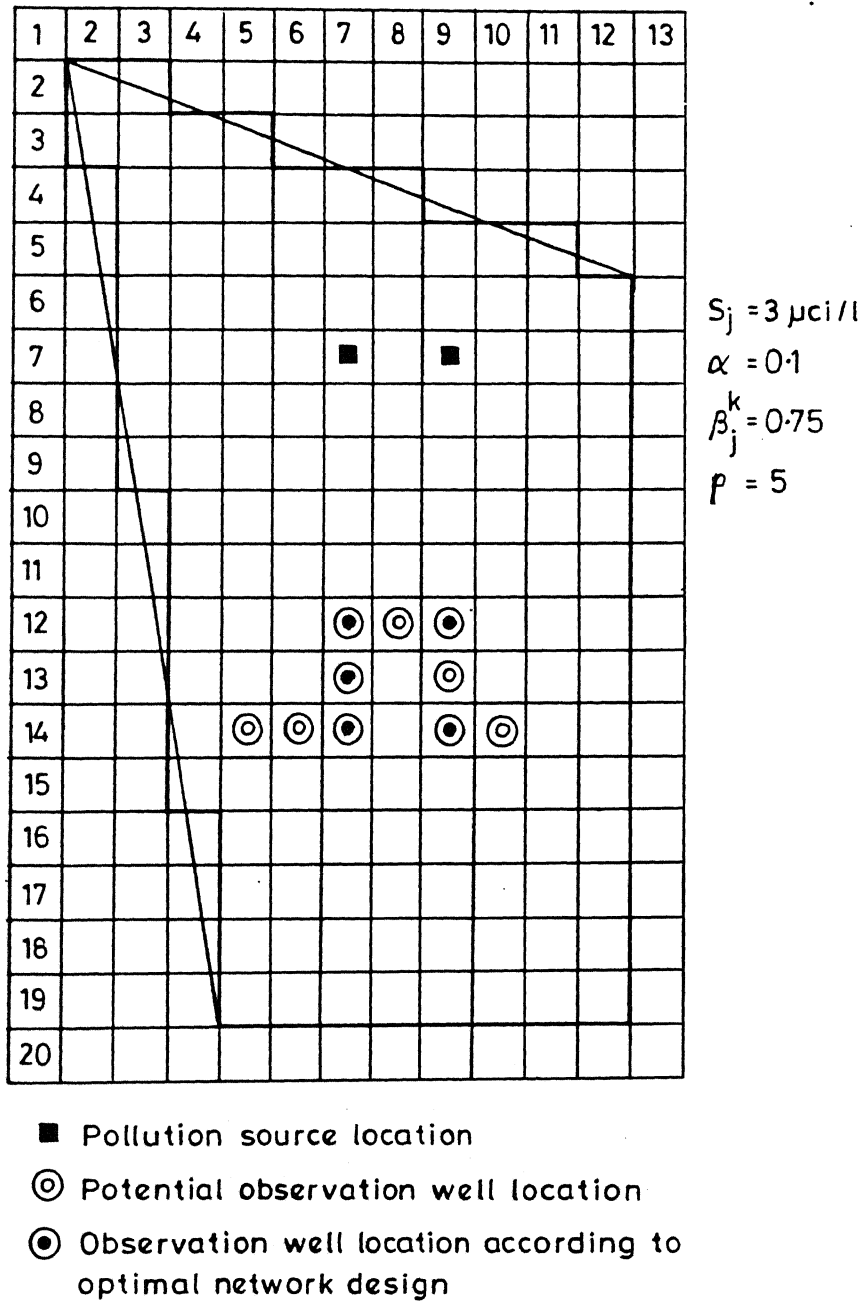


Figure 16 Optimal observation well locations obtained as solution to the model

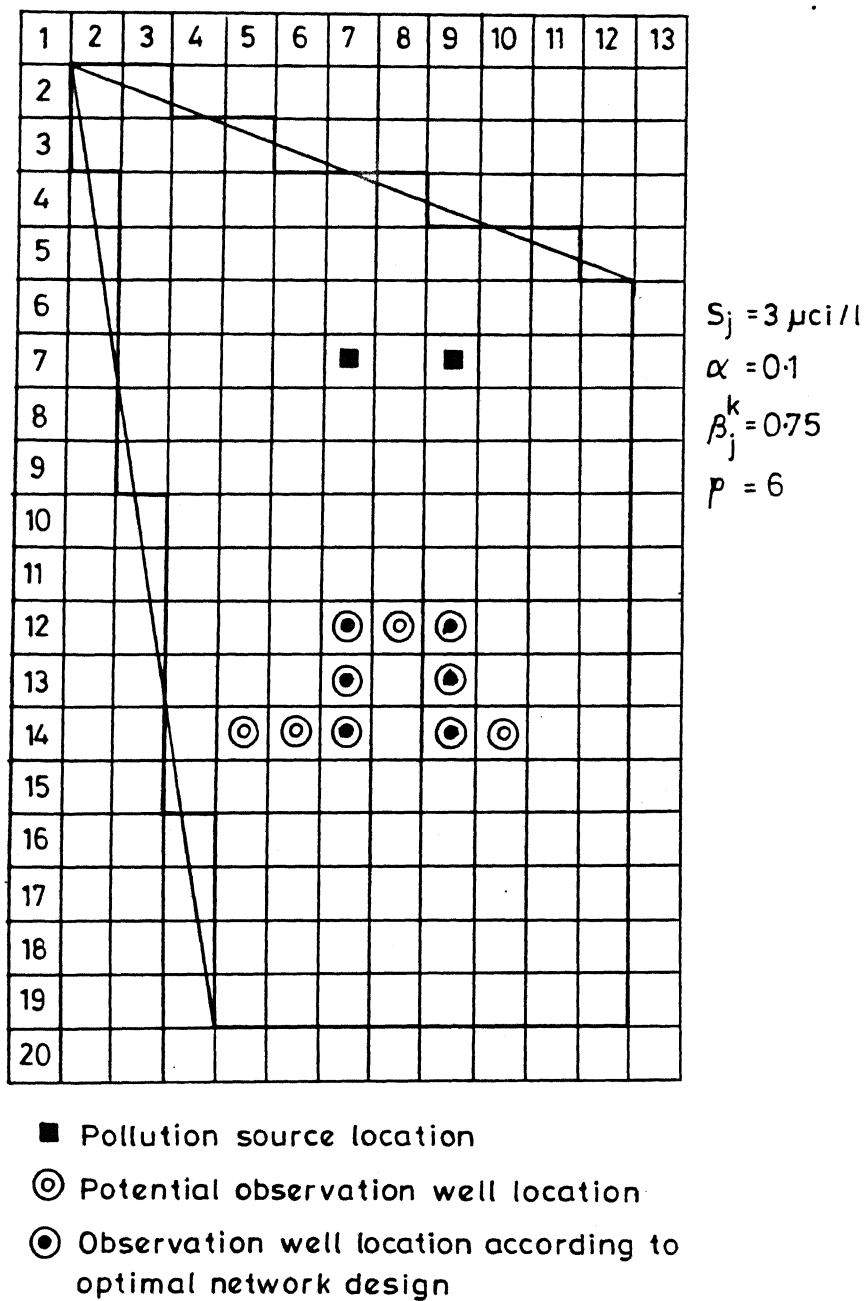


Figure 17 Optimal observation well locations obtained as solution to the model

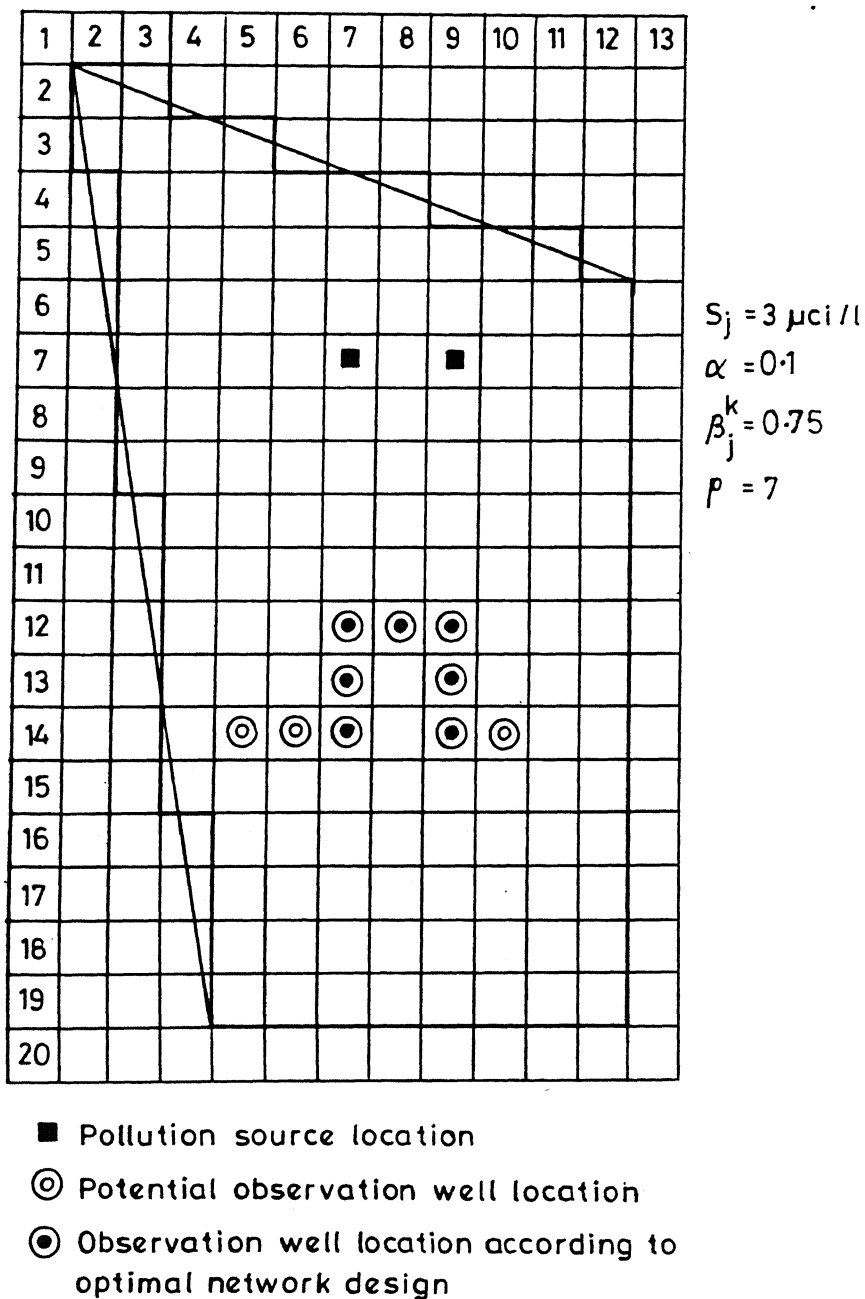


Figure 18 Optimal observation well locations obtained as solution to the model

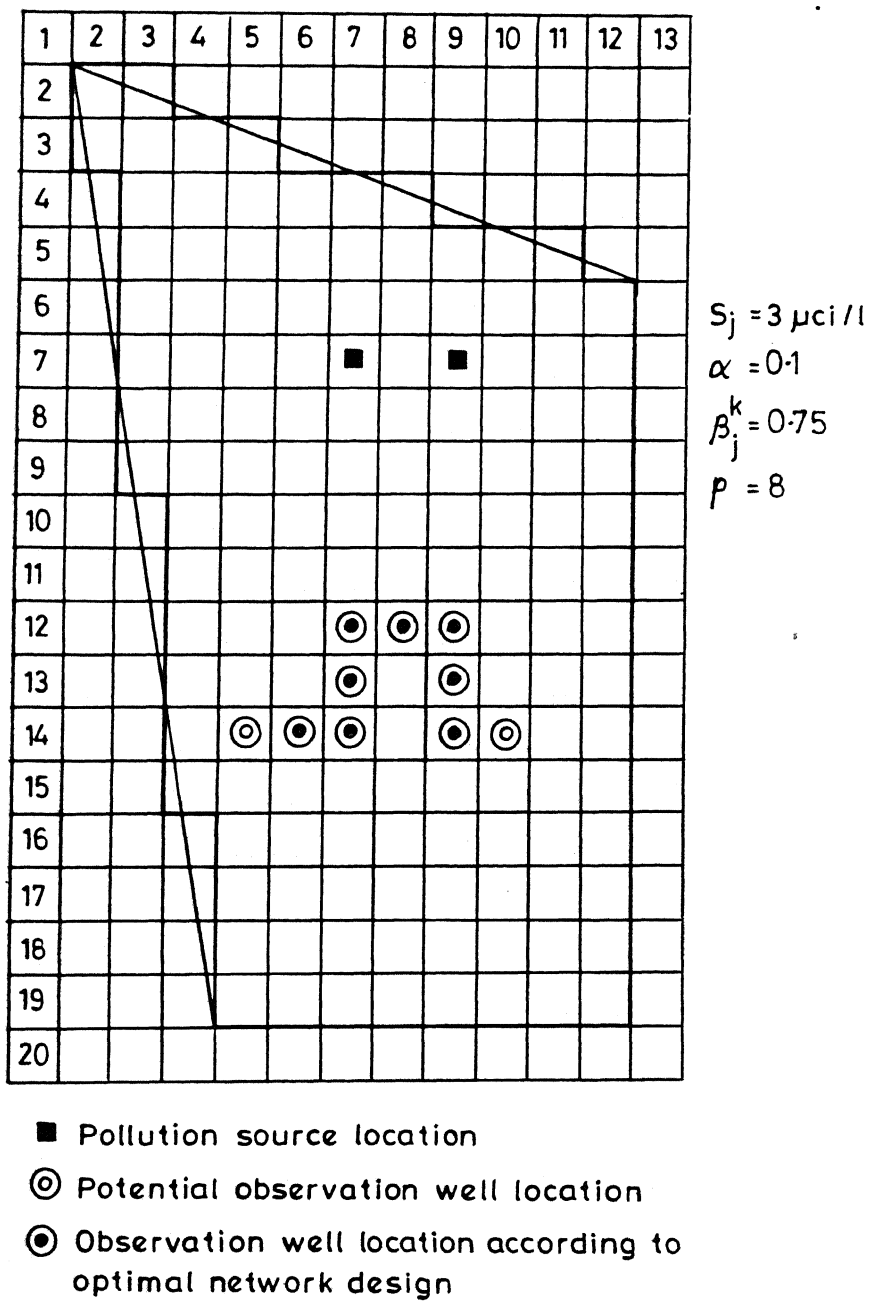
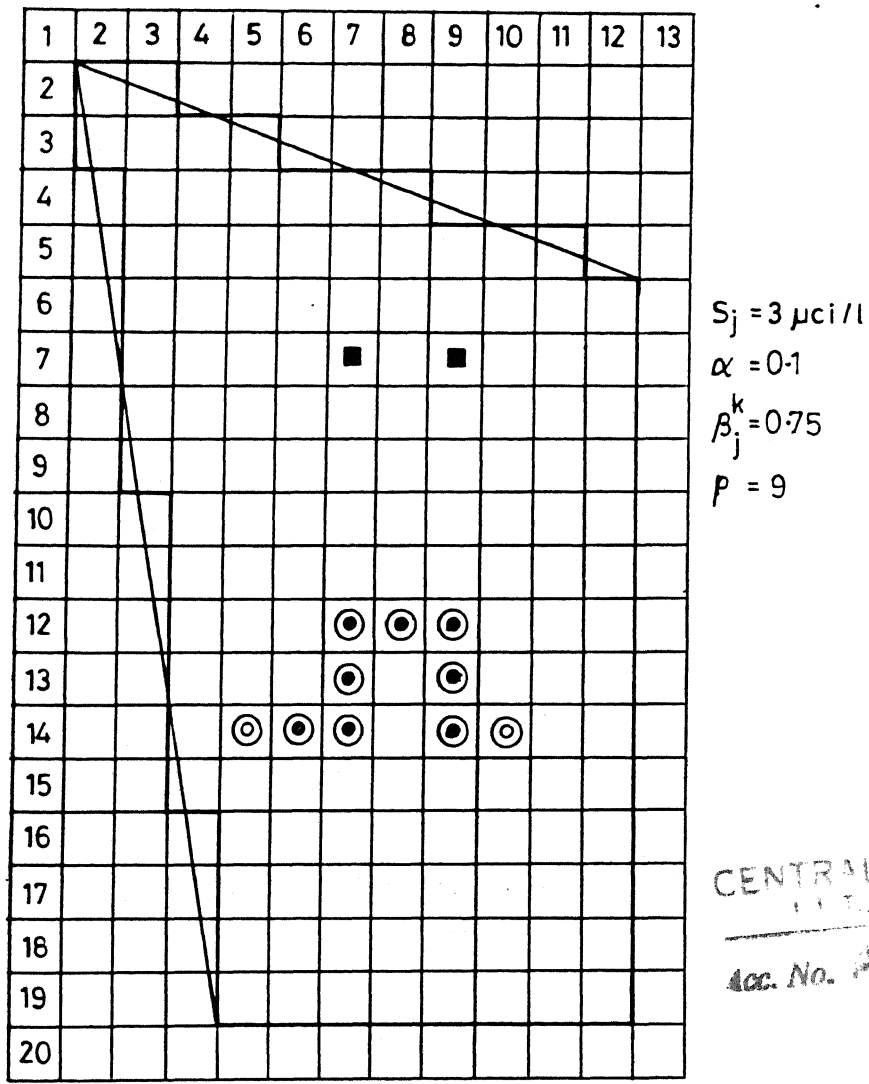


Figure 19 Optimal observation well locations obtained as solution to the model



- Pollution source location
- ⊙ Potential observation well location
- ⊙ Observation well location according to optimal network design

Figure 20 Optimal observation well locations obtained as solution to the model

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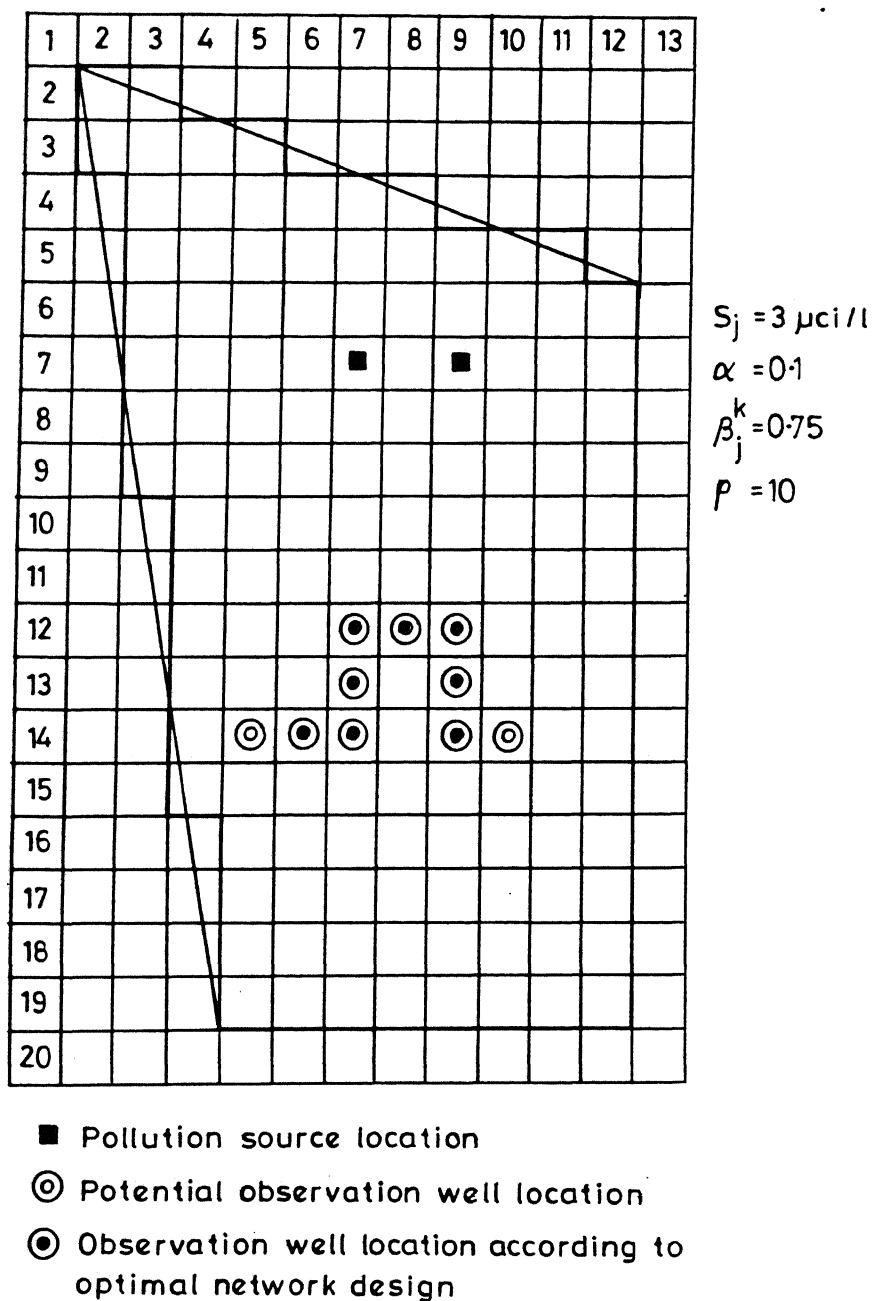


Figure 21 Optimal observation well locations obtained as solution to the model

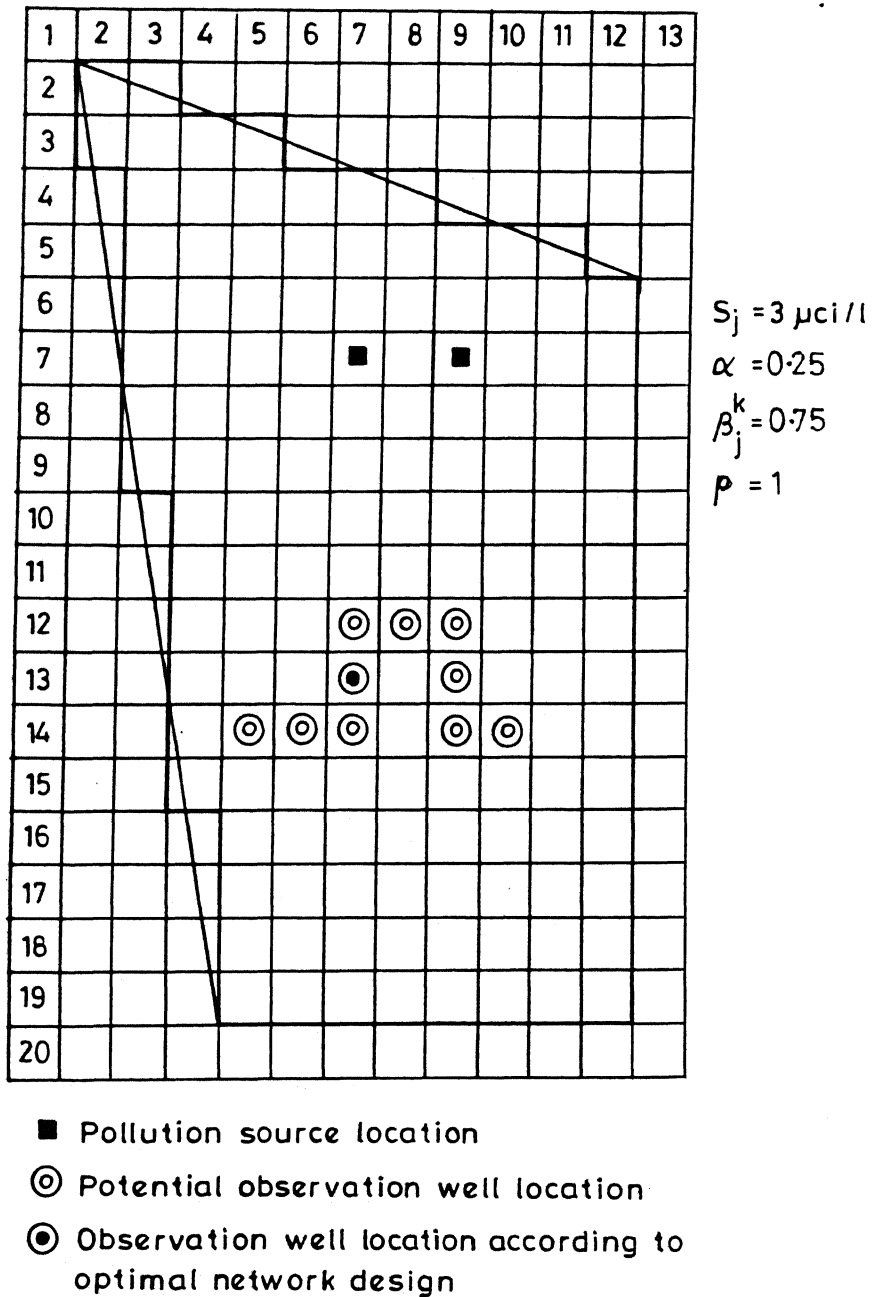


Figure 22 Optimal observation well locations obtained as solution to the model

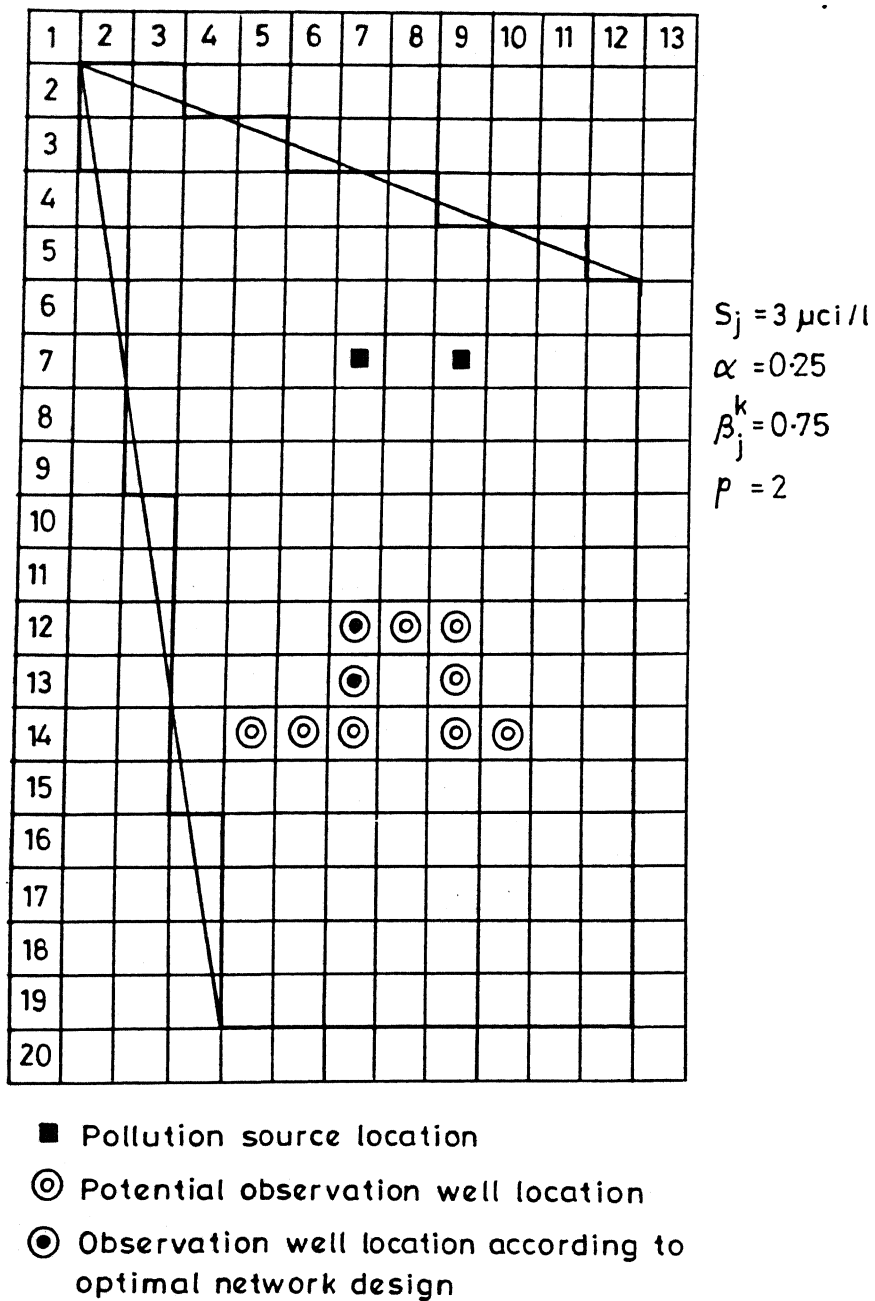


Figure 23 Optimal observation well locations obtained as solution to the model

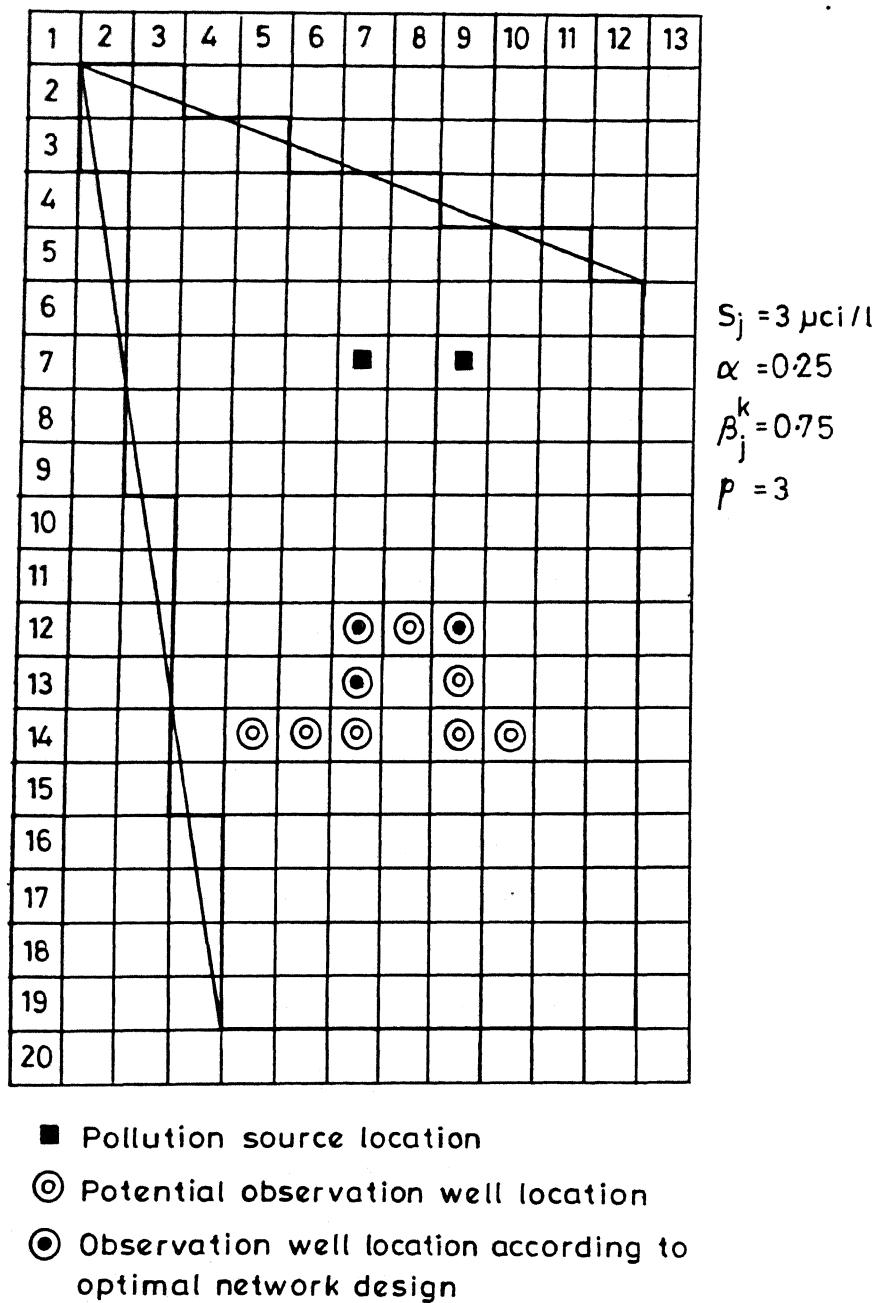


Figure 24 Optimal observation well locations obtained as solution to the model

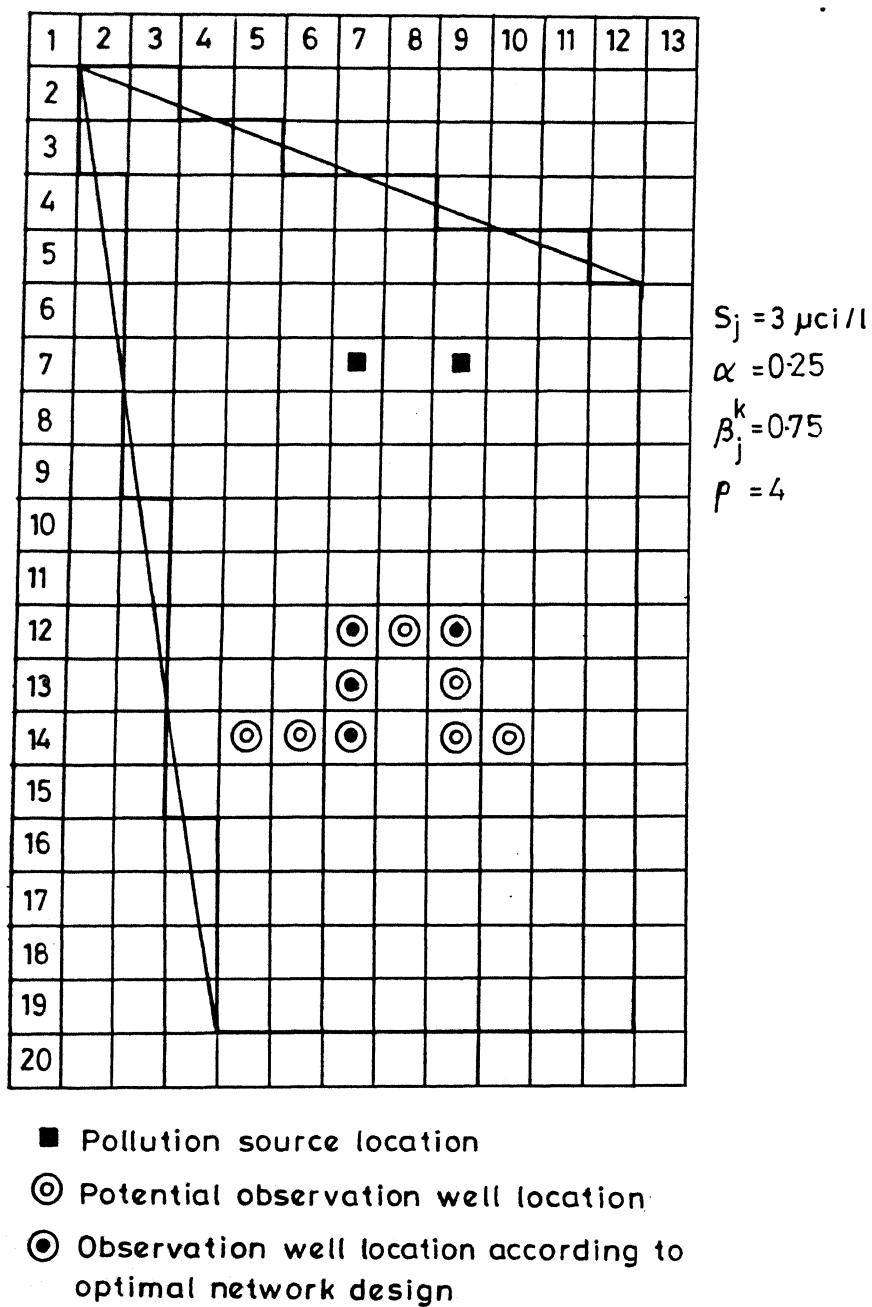


Figure 25 Optimal observation well locations obtained as solution to the model

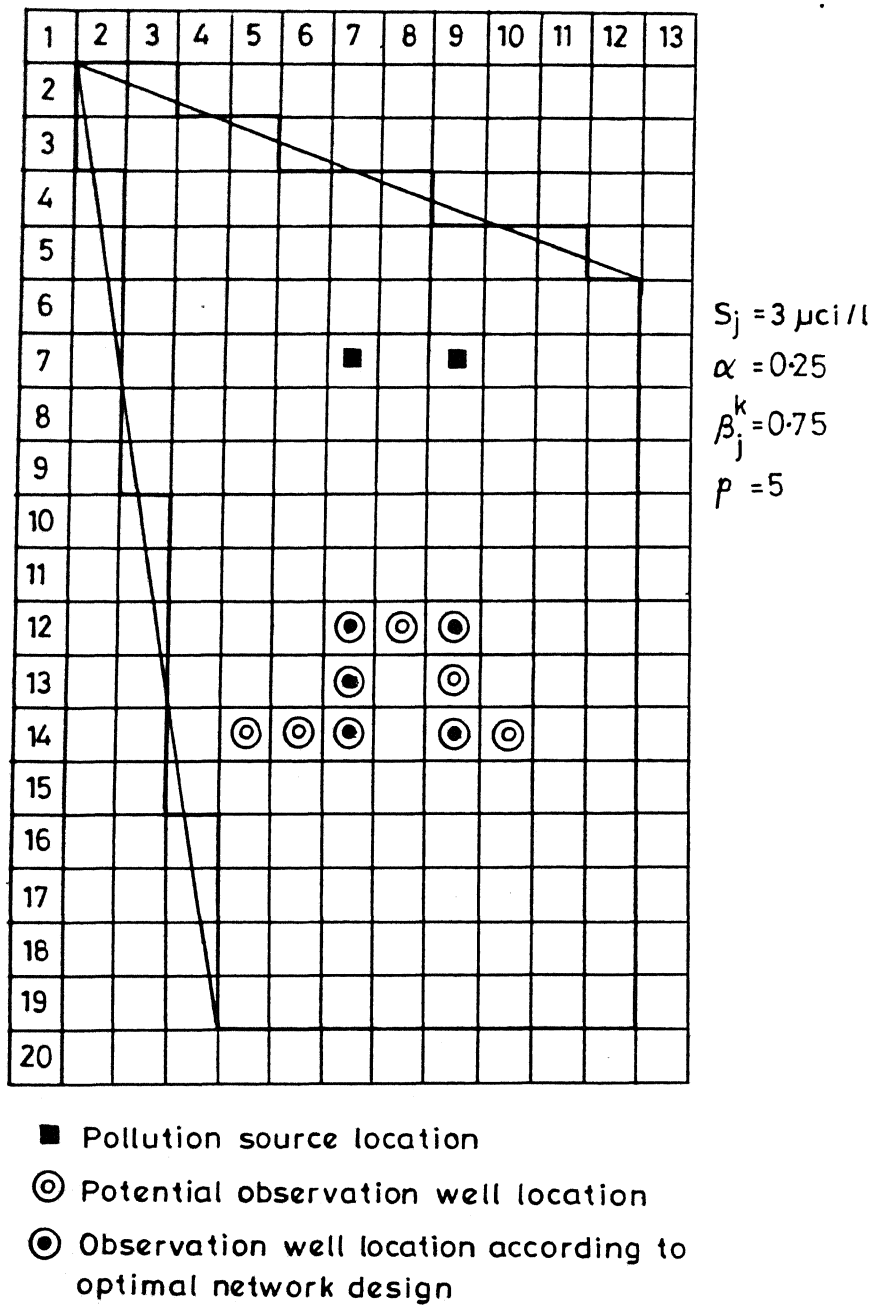


Figure 26 Optimal observation well locations obtained as solution to the model

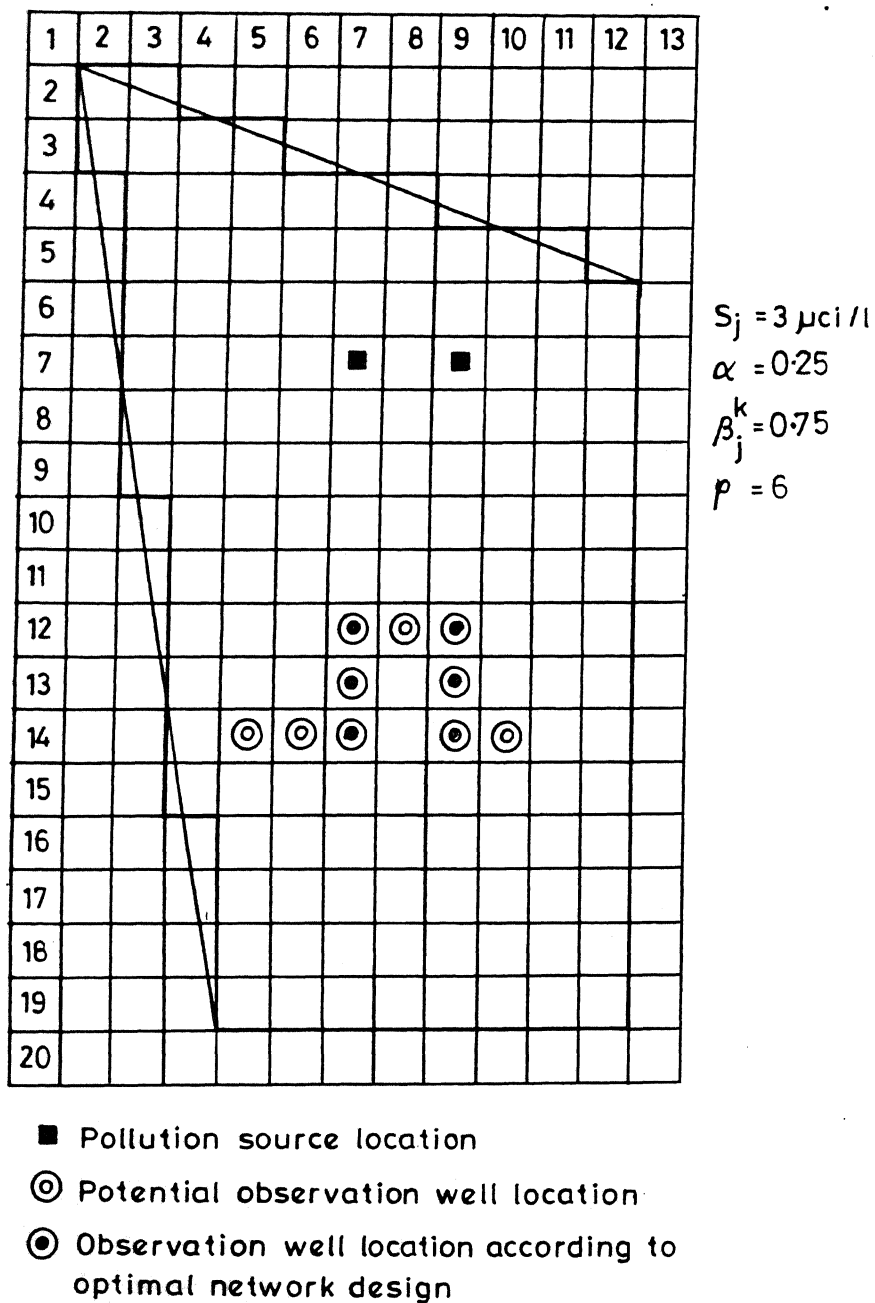
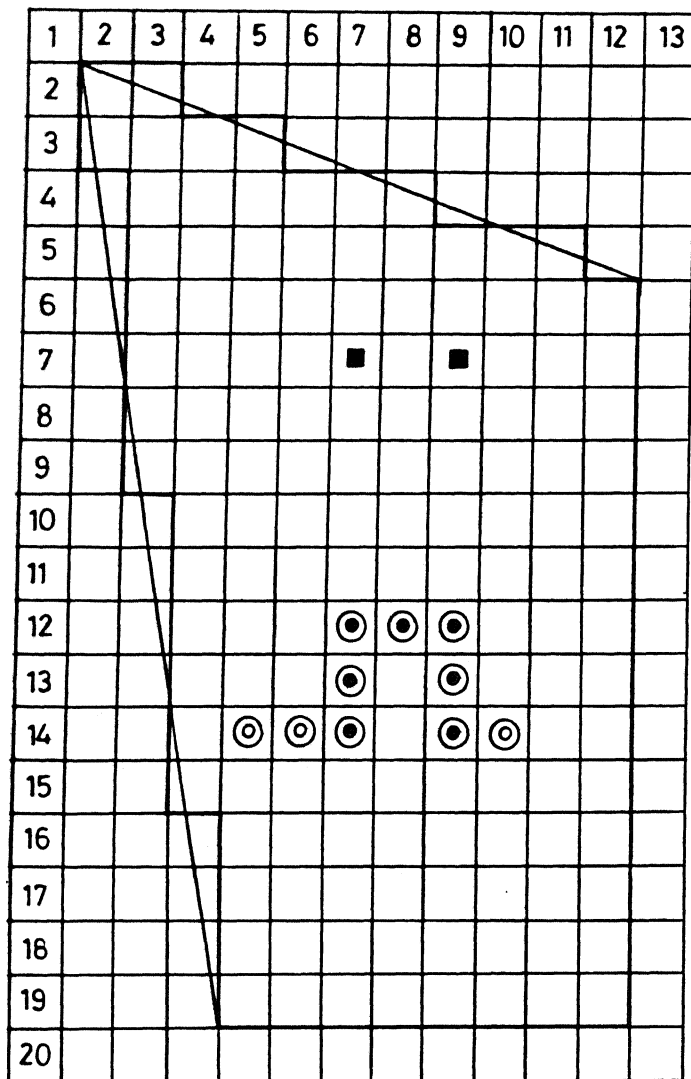


Figure 27 Optimal observation well locations obtained as solution to the model



$S_j = 3 \mu\text{ci/l}$

$\alpha = 0.25$

$\beta_j^k = 0.75$

$p = 7$

■ Pollution source location

⊙ Potential observation well location

⊙ Observation well location according to optimal network design

Figure 28 Optimal observation well locations obtained as solution to the model

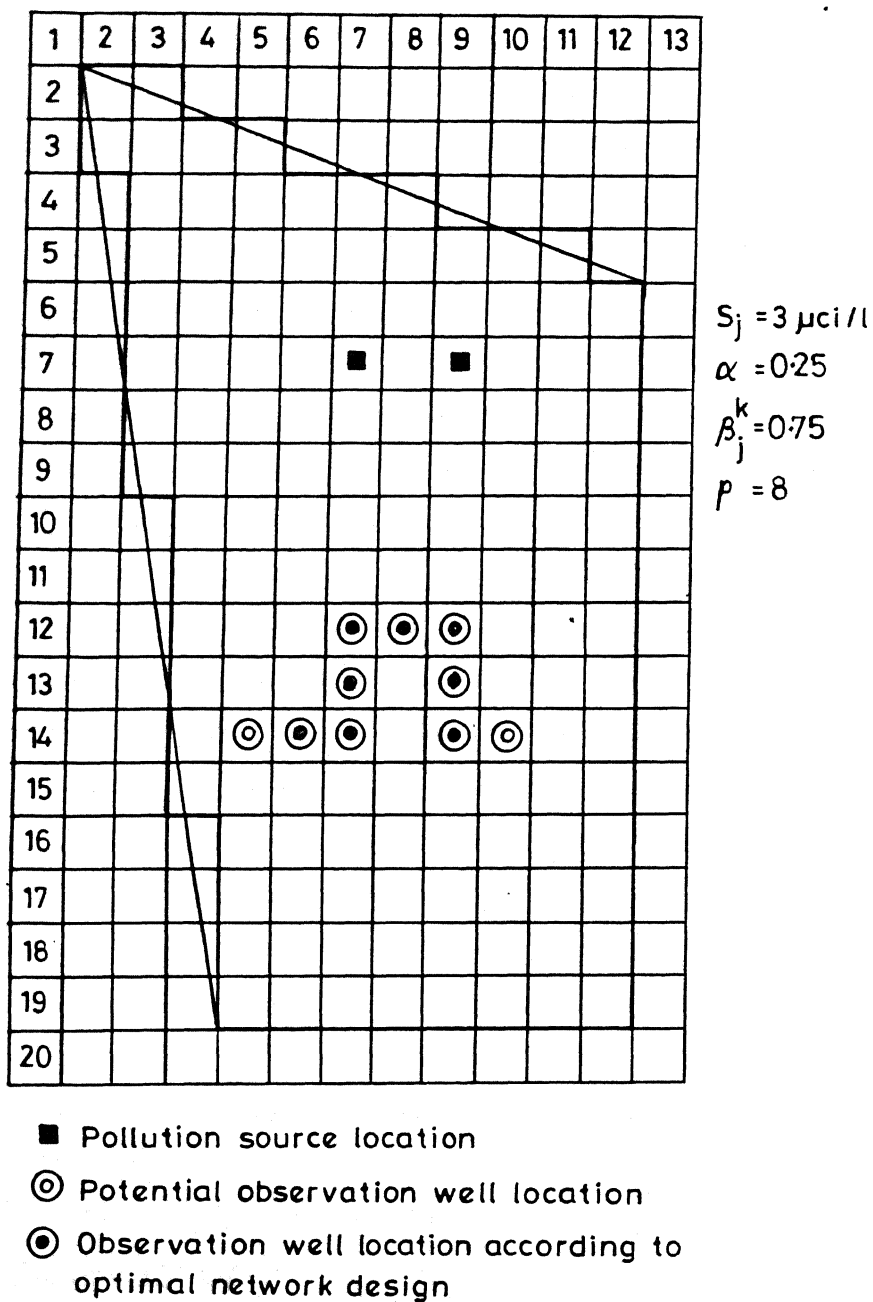


Figure 29 Optimal observation well locations obtained as solution to the model

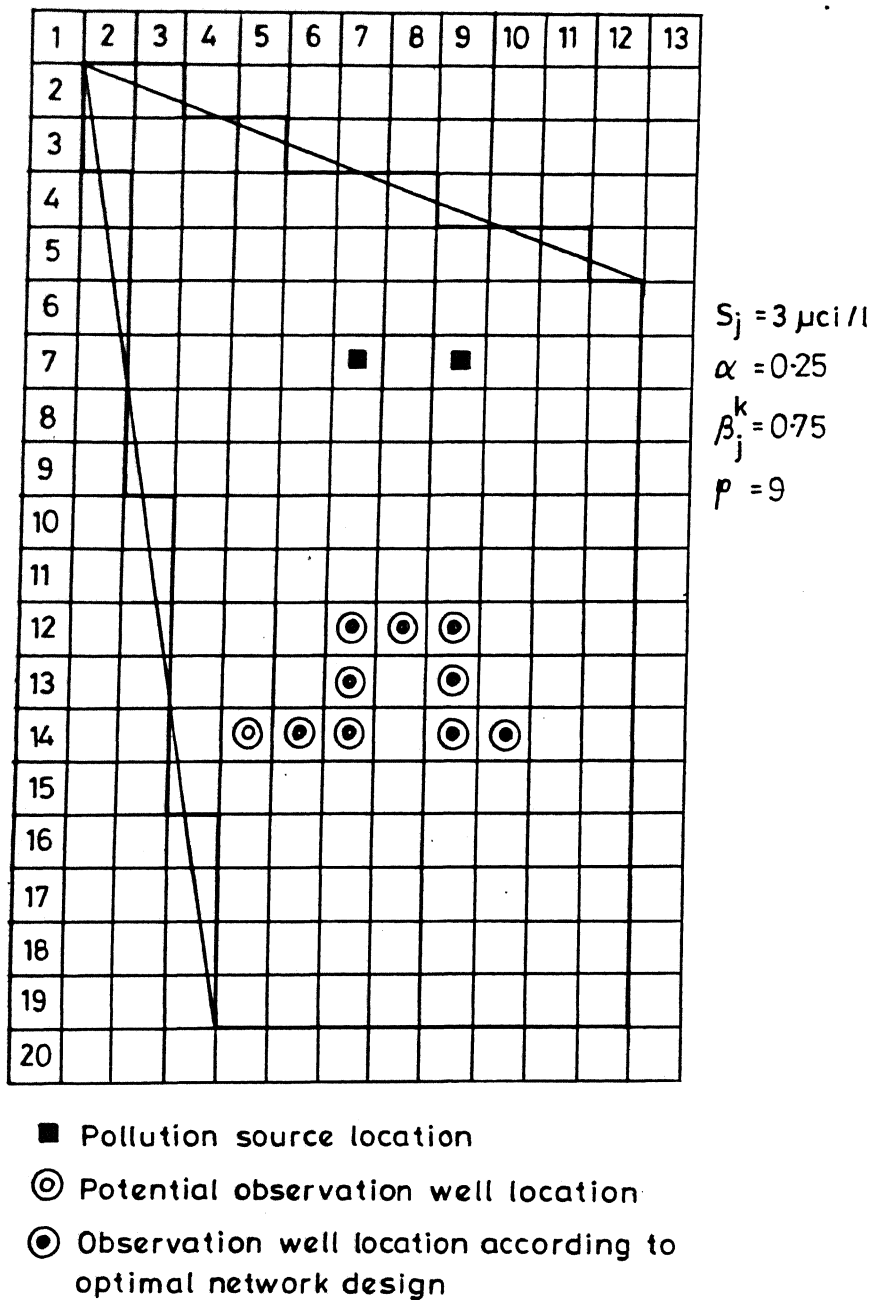


Figure 30 Optimal observation well locations obtained as solution to the model

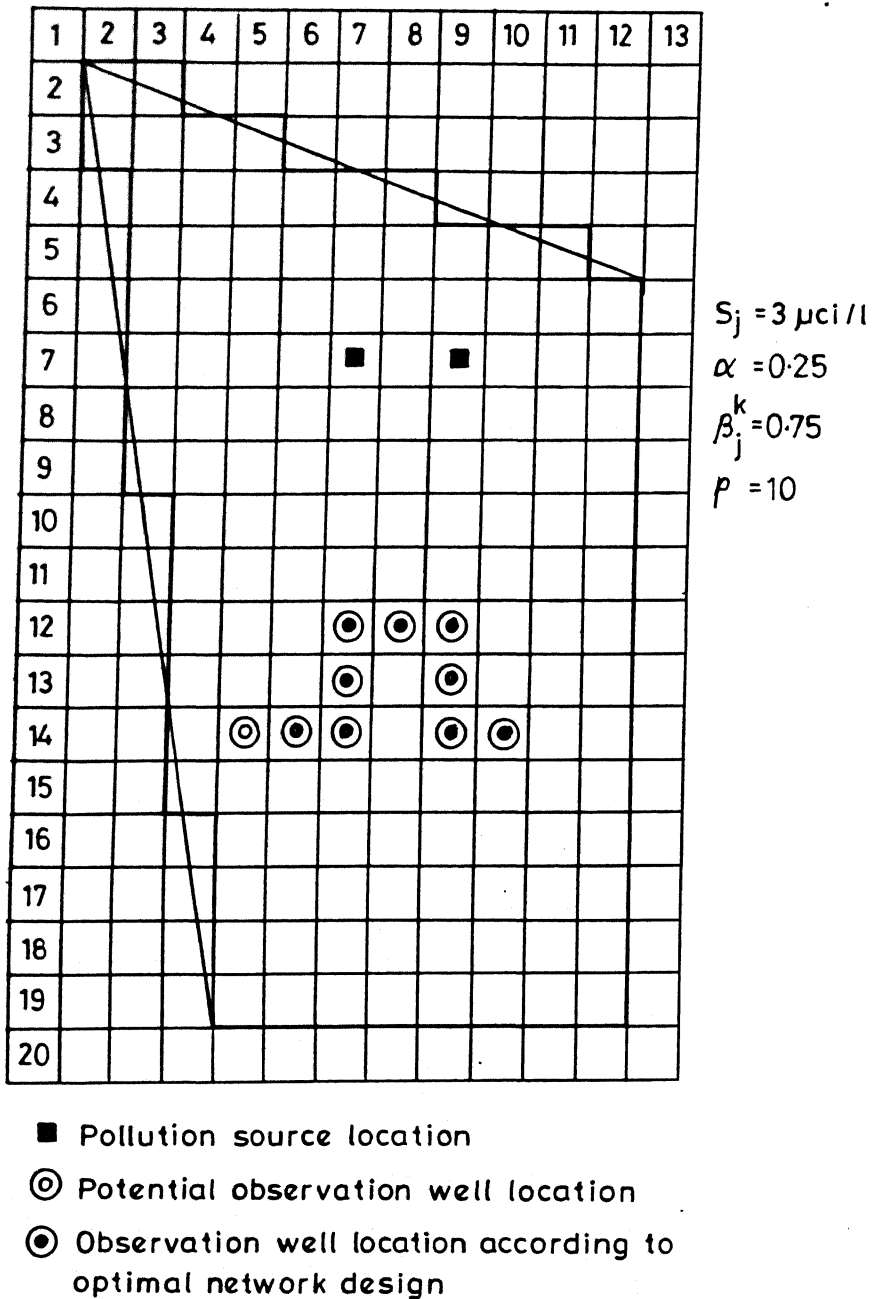


Figure 31 Optimal observation well locations obtained as solution to the model

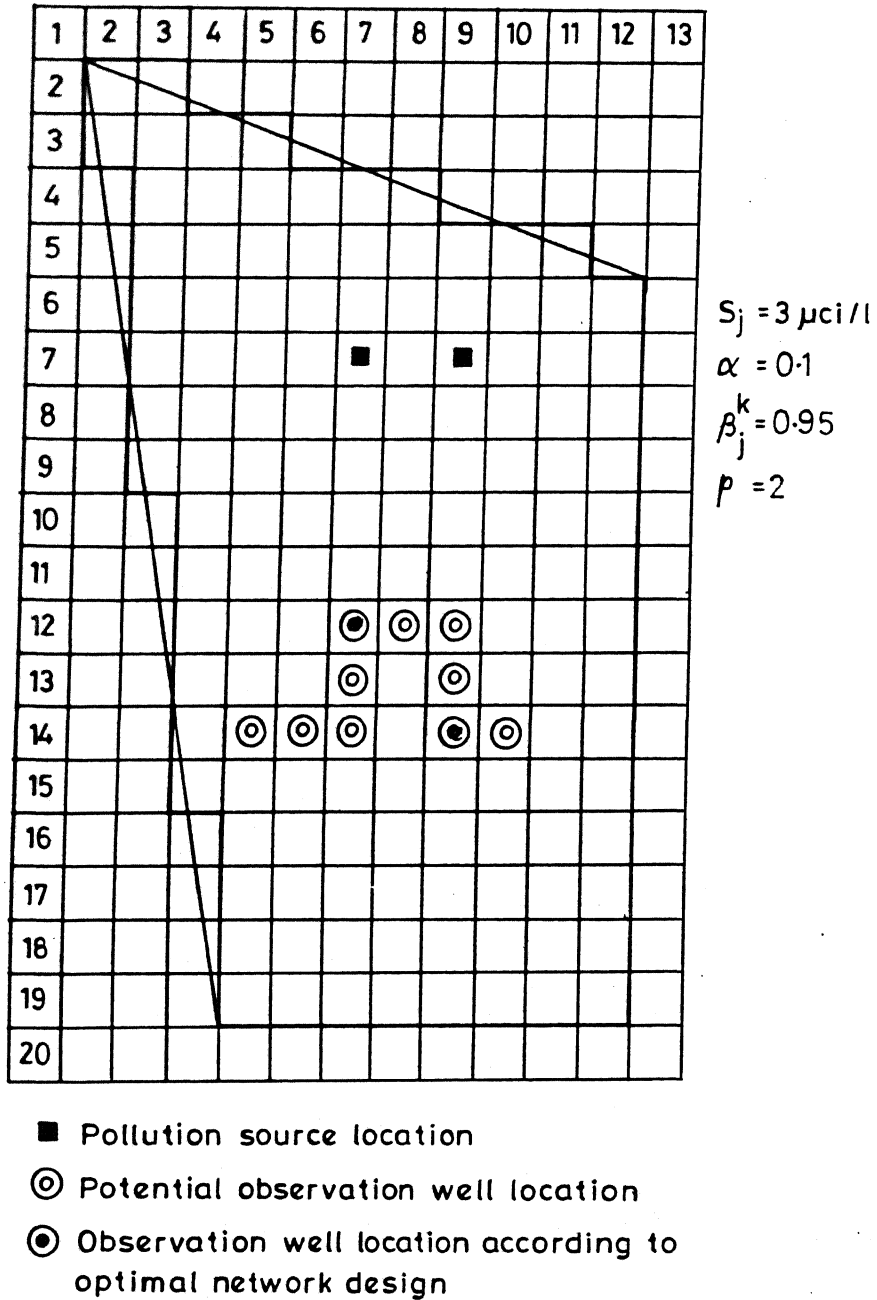


Figure 32 Optimal observation well locations obtained as solution to the model

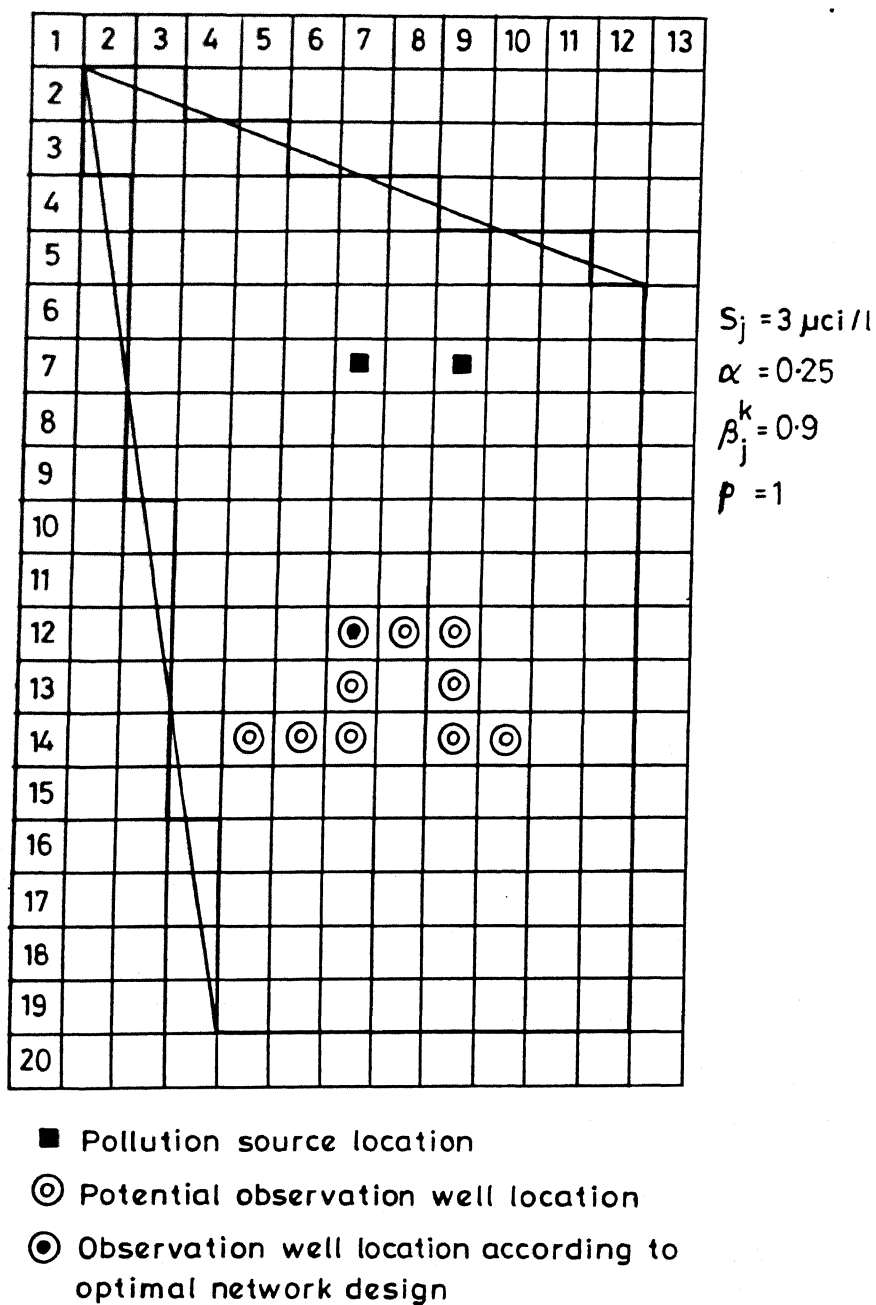


Figure 33 Optimal observation well locations obtained as solution to the model

values. The explicitly specified reliability levels are given by corresponding value of β_j^k .

A higher value of α signifies a greater degree of uncertainty in estimating or simulating the spatial and temporal distribution of concentrations. A higher value of β_j^k signifies, a more conservative prediction of these concentrations, for a given degree of uncertainty given by α .

A decision maker has to choose a particular value of α , depending on the perceived uncertainty in the transport modeling. A specified value of α denotes an overall subjective quantification of the uncertainties in modeling the transport process. A choice of β_j^k on the otherhand, will reflect a more conservative prediction of concentration for an already perceived degree of uncertainty. β_j^k values relate to the reliability of prediction in the sense that a higher β_j^k value will ensure that the probability of exceeding a predicted concentration is lower. A higher value of α signifies a higher degree of uncertainty in the modeling of transport. It is however, possible to obtain more realistic estimates of α values to be specified by using conventional methods of uncertainty analysis such as a first order uncertainty analysis (Tung, 1986).

The solution results demonstrate the feasibility of using this particular model linking a simulation and a chance constrained mixed integer programming optimization model for optimal design of groundwater quality monitoring network. These results also elucidate the significance of using different uncertainty measures and reliability values.

CHAPTER 4

SUMMARY AND CONCLUSION

4.1 SUMMARY

A mathematical model linking a groundwater pollution transport simulation model and a chance constrained optimization model explicitly considering uncertainties of transport simulation is developed for designing an optimal groundwater quality monitoring network. To illustrate the performance of this model a radioactive pollutant (Tritium, H^3) is considered. Therefore, this developed methodology is particularly applicable to radioactive waste disposal and groundwater quality monitoring. However, this method is easily applicable to other kinds of pollutants.

The simulation model provides the information about the pollutant transport with respect to time and space. In this study the groundwater transport simulation model has been combined with a statistical generation technique in an effort to incorporate uncertainties in the model parameters.

To provide a link between optimization and simulation model the response matrix approach has been utilized in which an external groundwater transport simulation model is used to develop unit response. An assemblage of the unit responses, a response matrix, is then used to simulate solute transport in groundwater,

for any given combination of pollution source location and magnitudes. Hence the problem of repeated simulation to provide input to optimization model is removed. In this approach, the response matrix itself is assumed to be uncertain.

A chance constrained optimization model is developed for an optimal design of groundwater quality monitoring network. The role of the chance constraints in the model is to introduce some degree of reliability in the predicted values of actual concentrations at specified locations. The optimization model incorporates the cumulative distribution function (CDF) of the actual concentration for each potential groundwater quality monitoring well location and for each specified management time period. The CDF's can be obtained by randomly varying the response matrix, that represents the response of the subsurface saturated zone for a given input of parameters.

The main objective of the chance constrained optimization model is to maximize the probability of detecting contamination at locations, where the standard is exceeded with due weightage given to its degree of exceedences. The exceedence values are computed in terms of the predicted values of concentration expressed as a function of specified reliabilities. The optimal design of monitoring well network restricts the total number of monitoring wells to a presepecified upper limit and at the same time takes into account the uncertainties of predicting solute transport in groundwater.

The performance of the developed model was evaluated for a number of scenarios with different degrees of uncertainties and different specified reliability values. These evaluations demonstrate the applicability of this model for design of groundwater quality monitoring networks, with inherent uncertainties in transport modeling.

4.2 ENGINEERING APPLICATION OF THE DEVELOPED METHODOLOGY

The methodology developed in this study is primarily useful for monitoring the temporal and spatial movement of a contaminant plume in groundwater. This detection is the first step in proper management of groundwater contamination. The optimal monitoring network ensures that the monitoring wells are installed at locations where these wells are able to detect contamination with high probabilities. Uncertainties present in the modeling of the contaminant plume movement require that the monitoring design network incorporate probabilities or reliabilities of detection. Given the upper limit on the number of monitoring wells to be installed generally based on economic considerations, the optimal design locates those sites where the resulting concentrations are probable to be very high. Thus it ensures an efficient network for monitoring while considering the uncertainties in parameter estimation, measurement errors, and other modeling uncertainties.

Depending on the actual purposes of groundwater withdrawal, such as domestic water supply, irrigation water supply, industrial uses and others. This model is capable of using different allowable standards for contaminant concentrations at different locations. Therefore, if for example, groundwater at a location

is being used for drinking purposes, a lower value of allowable or standard concentration can be used at that location, to ensure more efficient monitoring at that location. Also, different weights can be introduced in the objective function, to reflect the importance given to the exceedence of a given standard at a given location.

In particular, this methodology will be useful in monitoring the effects of radioactive pollutant disposals from nuclear power plants. Also, the optimal monitoring network can be used to detect and subsequently manage contamination of the groundwater due to accidental disposal of radioactive wastes.

4.3 CONCLUSIONS

1. A mathematical model linking a groundwater solute transport simulation model and a chance constrained optimization model is developed. The optimization model explicitly considers uncertainties of transport simulation and incorporates specified reliabilities of predicting the actual concentration in time and space.
2. The model is evaluated for different degree of uncertainties in the modeling process by introducing CDF's of actual concentrations as constraints in the optimization model.
3. The solution results show that the optimal well locations are significantly dependent on the degree of uncertainties and the specified reliability values.

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APPENDIX - [A]

**FORTRAN Programme for
Statistical perturbation of the
[R] matrix.**

C
C

```
STATISTICAL PERTURBATION OF THE [R] MATRIX
*****
DIMENSION S(10),C(1000)
DIMENSION F(1000,10),CN(1000,10),CN1(1000,10)
OPEN(UNIT=50,FILE='dhi.man.prn')
OPEN(UNIT=31,FILE='sun.dat')
OPEN(UNIT=31,FILE='H2')
OPEN(UNIT=32,FILE='H3')
OPEN(UNIT=30,FILE='H1')
OPEN(UNIT=23,FILE='H4')
OPEN(UNIT=34,FILE='H5')
OPEN(UNIT=35,FILE='H6')
OPEN(UNIT=36,FILE='H7')
OPEN(UNIT=37,FILE='H8')
OPEN(UNIT=38,FILE='H9')
OPEN(UNIT=39,FILE='H10')
ALPHA=0.25
RMEAN=0.0
IP=17954
DO I=1,1000
  READ(50,*)(R(I,J),J=1,8)
ENDDO
READ(31,*)(S(I),I=1,8)
DO 200 M=1,100
  DO I=1,1000
    DO J=1,8
      SIGMA=R(I,J)*ALPHA
      CALL SPAND(IP)
      R1=RAND()
      R2=RAND()
      Y=(-2.*ALOG(R1))*0.5*COS(6.283*R2)
      CN(I,J)=SIGMA*Y+RMEAN
      CN1(I,J)=R(I,J)+CN(I,J)
      IF(CN1(I,J).LT.0.0) GO TO 15
      IP = IP+100
    ENDDO
  ENDDO
  DO I =1,1000
    C(I) =0.0
    DO 20 J=1,8
      C(I)=C(I)+CN1(I,J)*S(J)
    CONTINUE
  ENDDO
  WRITE(30,*)(C(I),I=10,100,9)
  WRITE(21,*)(C(I),I=110,200,9)
  WRITE(22,*)(C(I),I=210,300,9)
  WRITE(23,*)(C(I),I=310,400,9)
  WRITE(34,*)(C(I),I=410,500,9)
  WRITE(35,*)(C(I),I=510,600,9)
  WRITE(36,*)(C(I),I=610,700,9)
  WRITE(37,*)(C(I),I=710,800,9)
  WRITE(38,*)(C(I),I=810,900,9)
  WRITE(39,*)(C(I),I=910,1000,9)
  IP=IP+100
200 CONTINUE
STOP
END
```

15

20

200